Pancreatic cancer drug discovery based upon (+)-grandifloracin

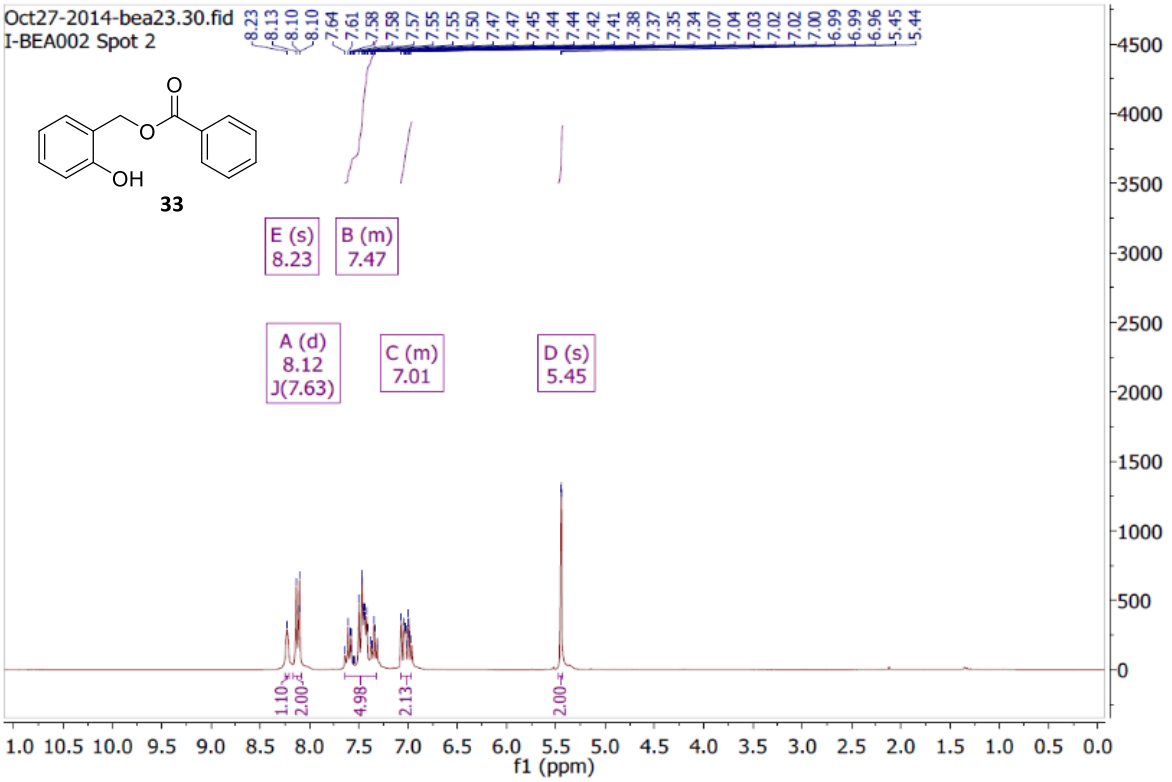
Alexander, Benjamin

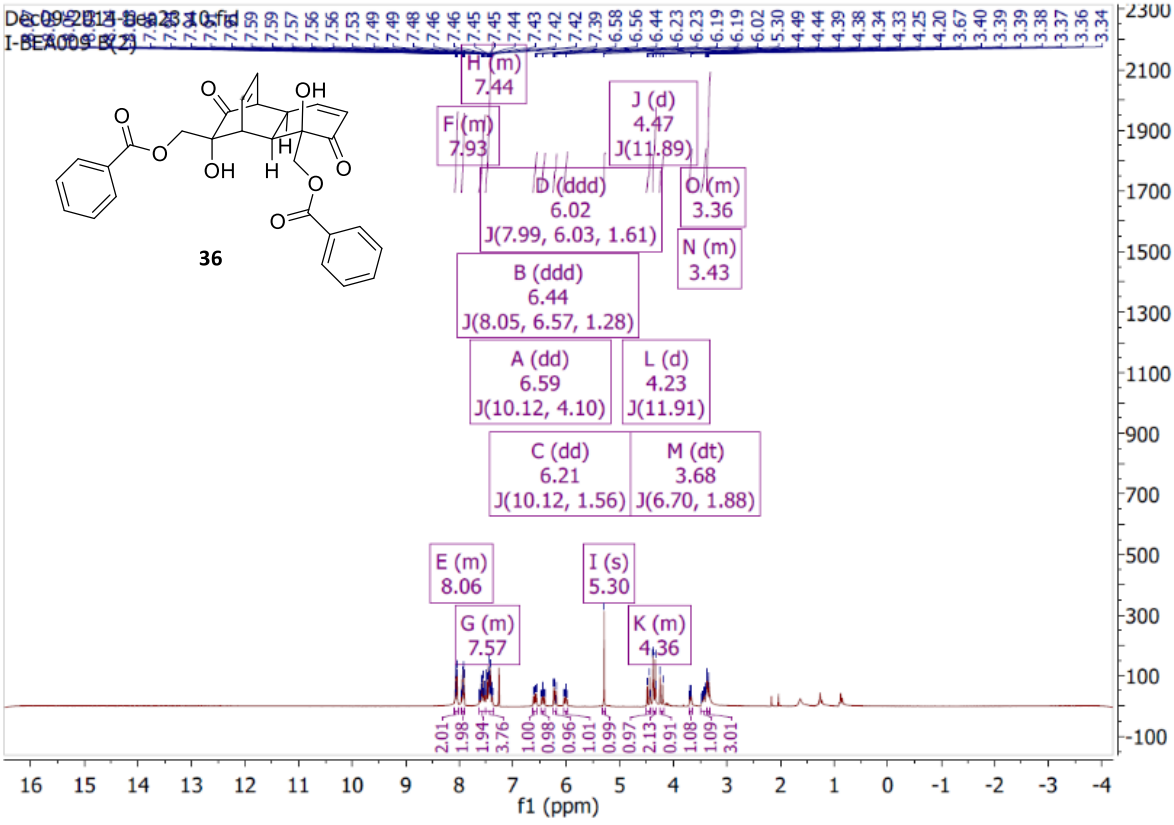
Award date:
2019

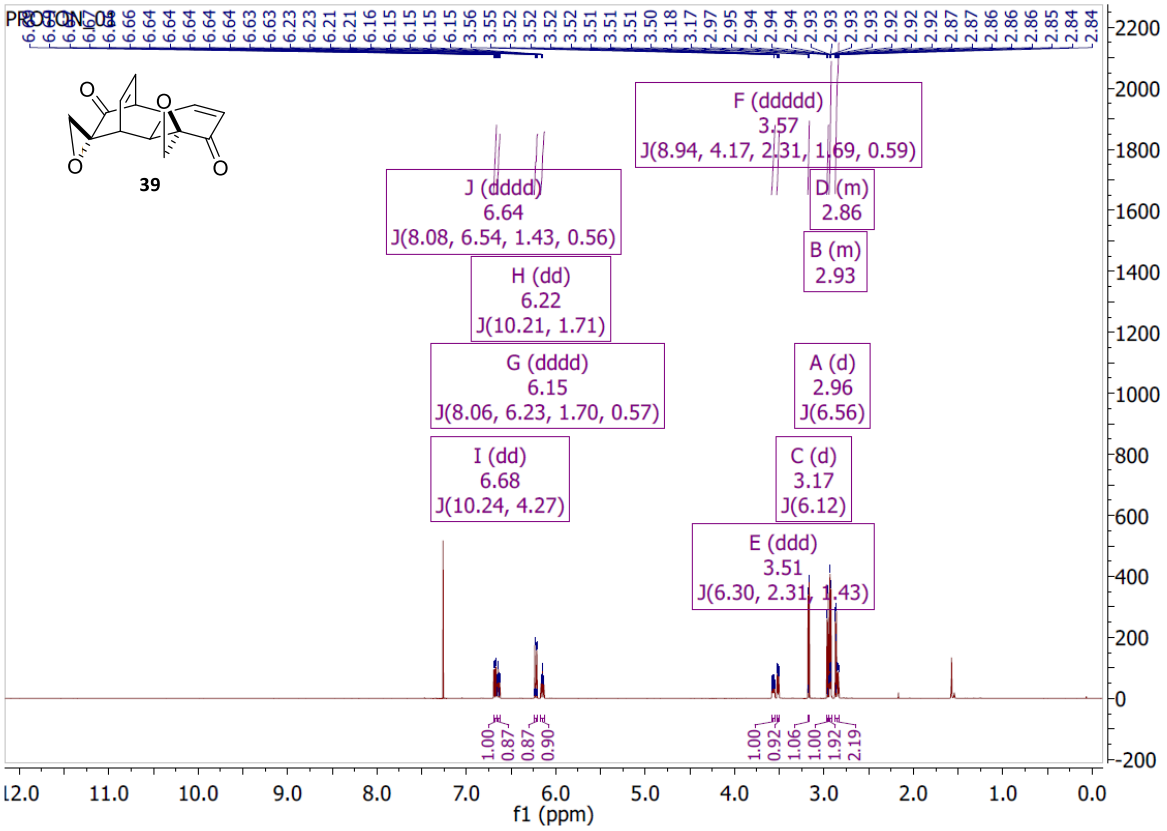
Awarding institution:
University of Bath

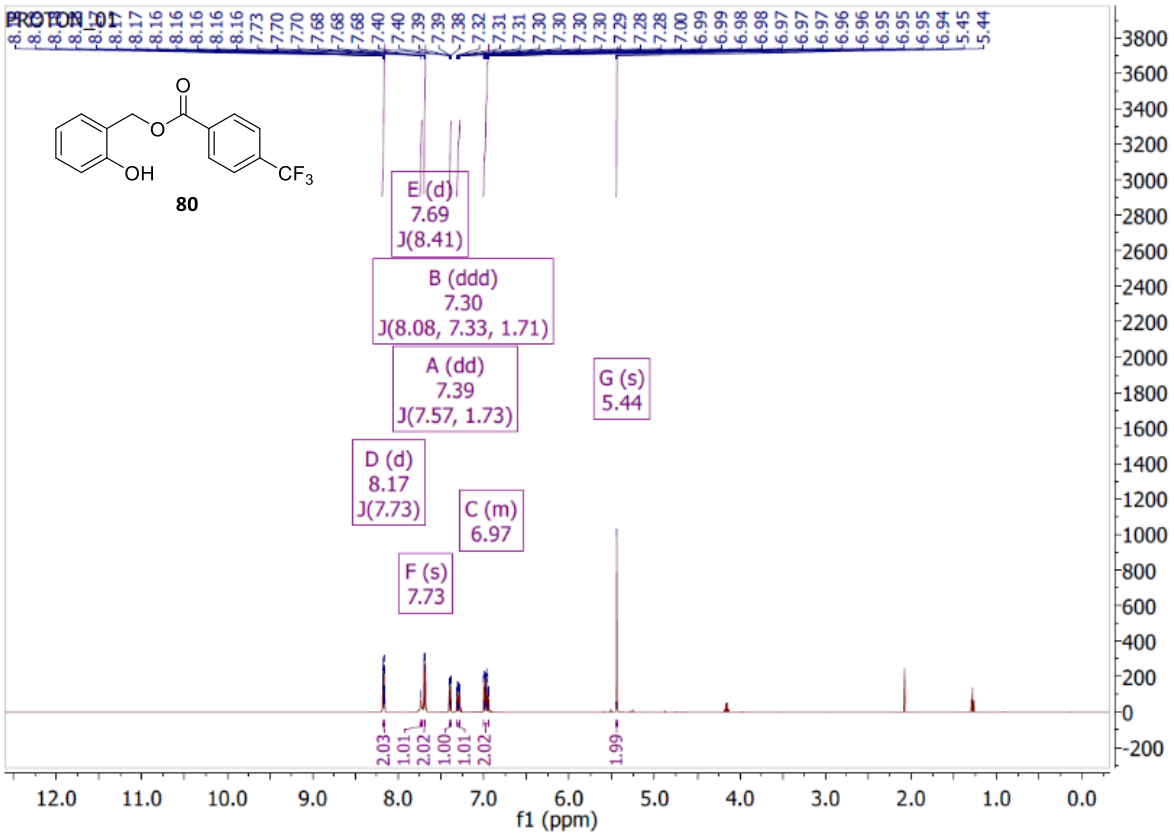
7.0: Appendix

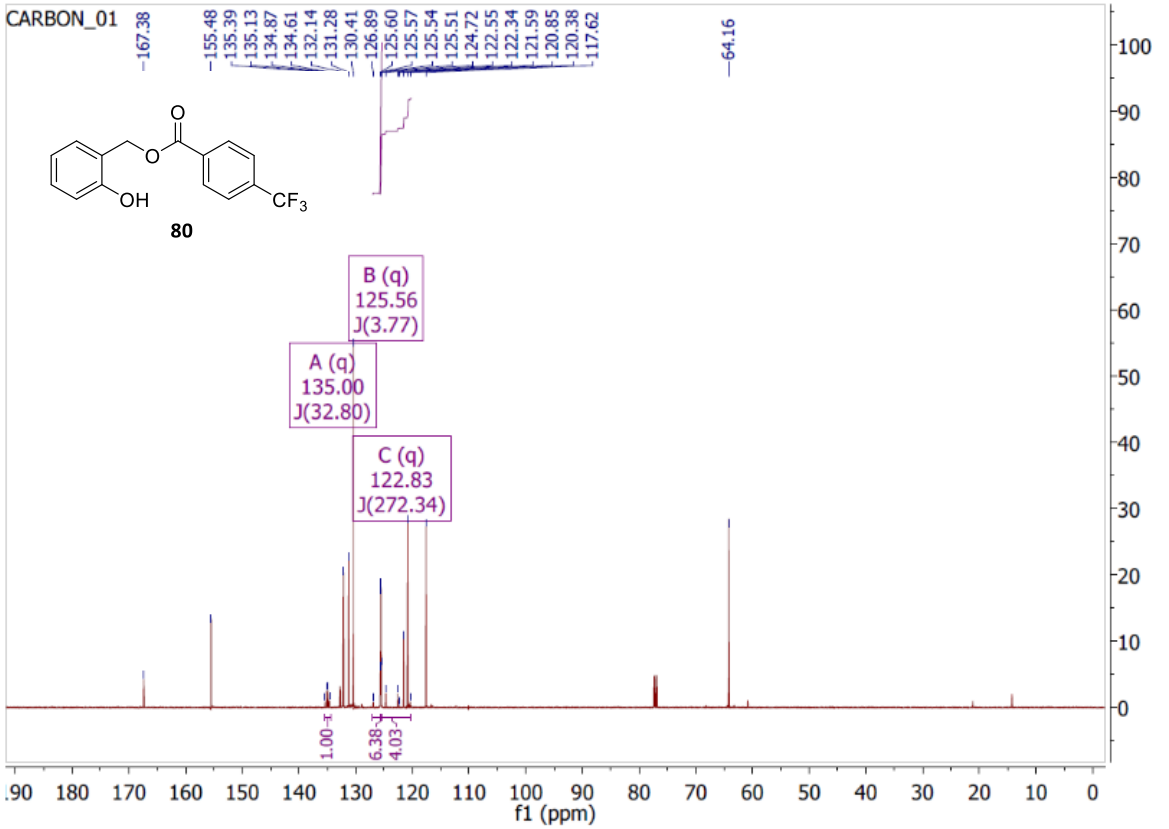
7.1: Spectroscopy and spectrometry data

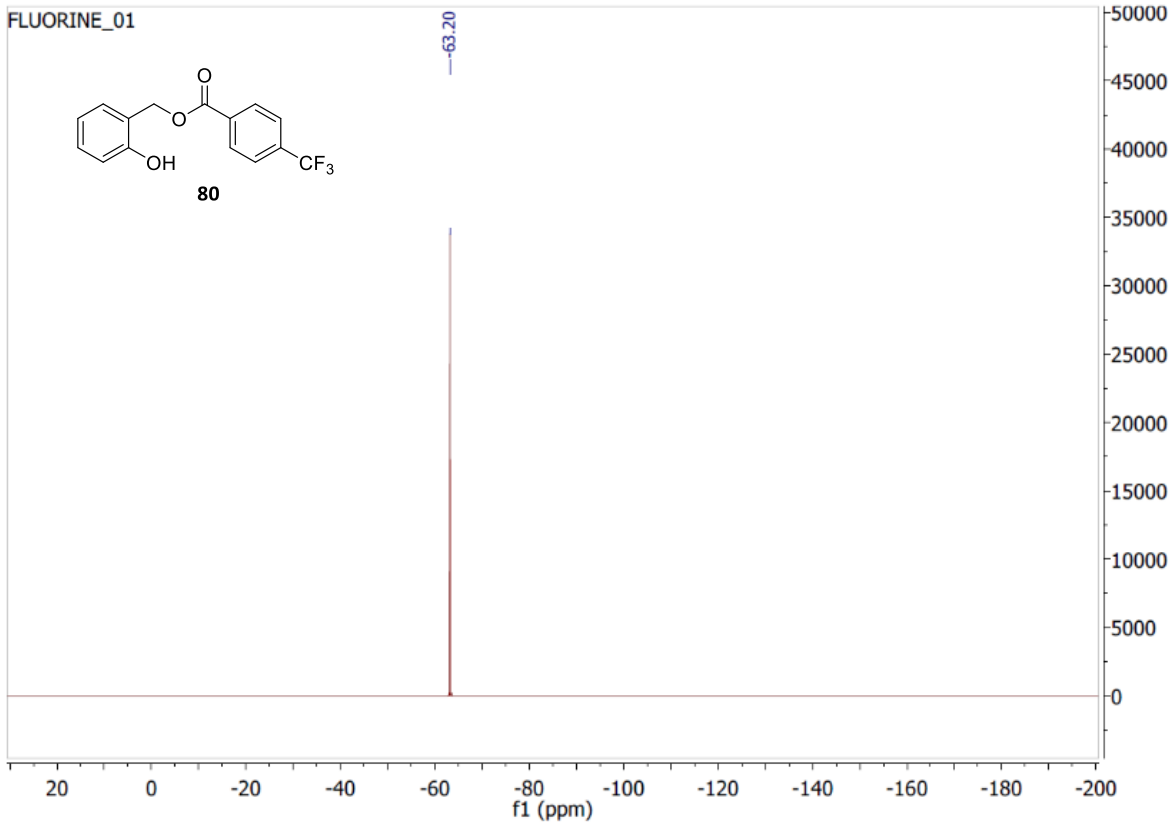


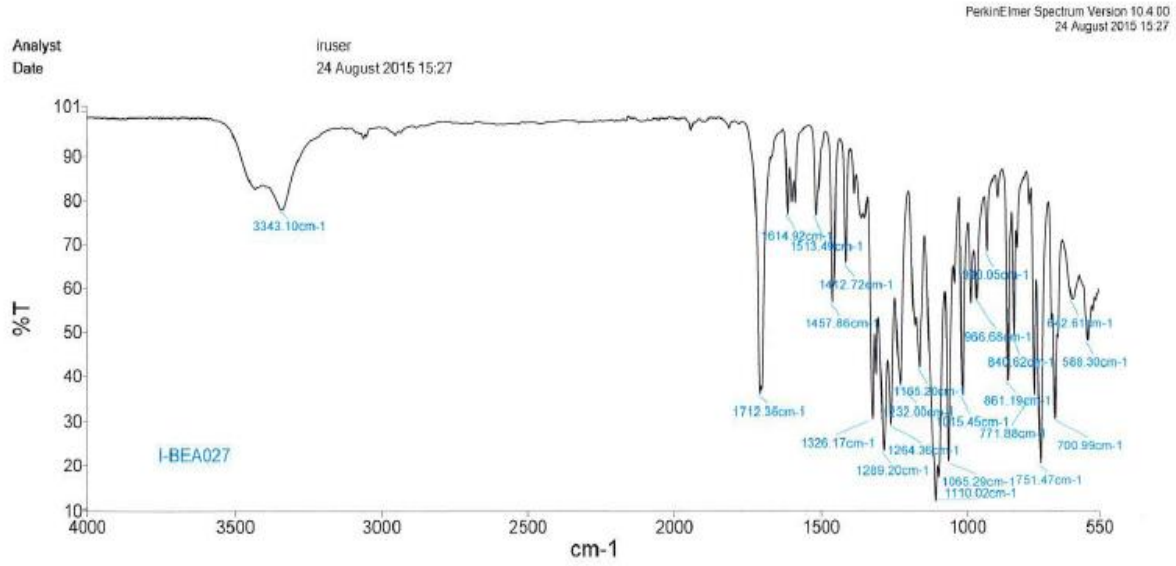



PROTON_03
39
F (ddddd)
3.57
J(8.94, 4.17, 2.31, 1.69, 0.59)
J (dddd)
6.64
J(8.08, 6.54, 1.43, 0.56)
D (m)
2.86
B (m)
2.93
H (dd)
6.22
J(10.21, 1.71)
G (dddd)
6.15
J(8.06, 6.23, 1.70, 0.57)
A (d)
2.96
J(6.56)
I (dd)
6.68
J(10.24, 4.27)
C (d)
3.17
J(6.12)
E (ddd)
3.51
J(6.30, 2.31, 1.43)
f1 (ppm)


PROTON_01
80
OH
CF3
E (d)
7.69
J(8.41)
B (ddd)
7.30
J(8.08, 7.33, 1.71)
A (dd)
7.39
J(7.57, 1.73)
G (s)
5.44
D (d)
8.17
J(7.73)
C (m)
6.97
F (s)
7.73
f1 (ppm)


CARBON_01
167.38
155.48
135.39
135.13
134.87
134.61
132.14
131.28
130.41
126.89
125.60
125.57
125.54
125.51
124.72
122.55
122.34
121.59
120.85
120.38
117.62
64.16
OH
CF3
80
B (q)
125.56
J(3.77)
A (q)
135.00
J(32.80)
C (q)
122.83
J(272.34)
1.00
6.38
4.03
f1 (ppm)


FLUORINE_01
63.20
OH
CF3
80
f1 (ppm)



Sample Name	Description	Quality Checks
I-BEA027 B (1)	Sample 1157 By iruser Date Thursday, May 07 2015	The Quality Checks do not report any warnings for the sample.

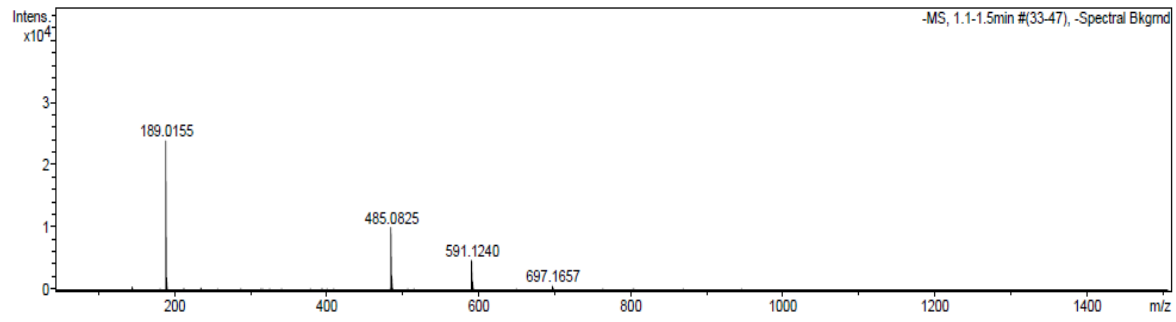
Mass Spectrum SmartFormula Report

Analysis Info

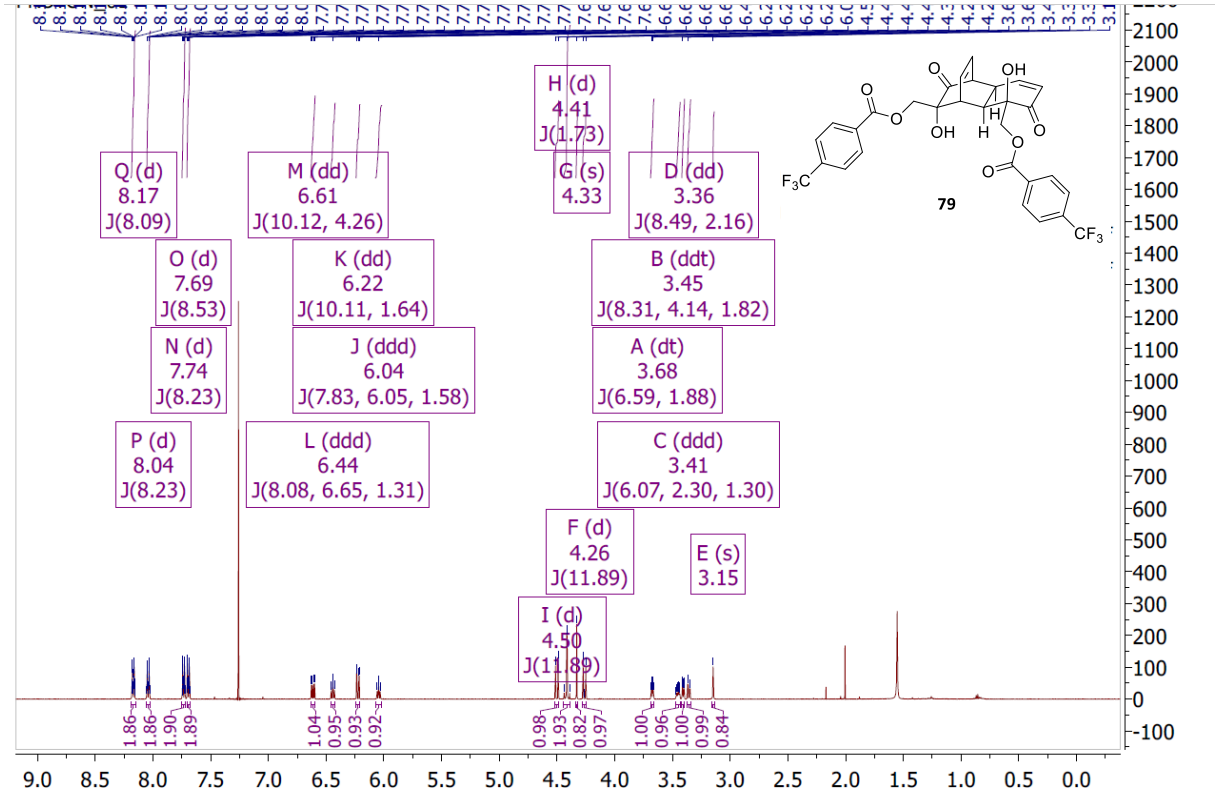
Analysis Name	C:\Documents and Settings\Administrator\My Documents\Ben\ba_sel_I-BEA027 B_343733_77_01_48134.d	Acquisition Date	5/7/2015 3:43:45 PM
Method	Confirm Formula Negative 50to1500 loop inj.m	Operator	admin
Sample Name	ba_sel_I-BEA027 B_343733	Instrument / Ser#	micrOTOF 161
Comment			

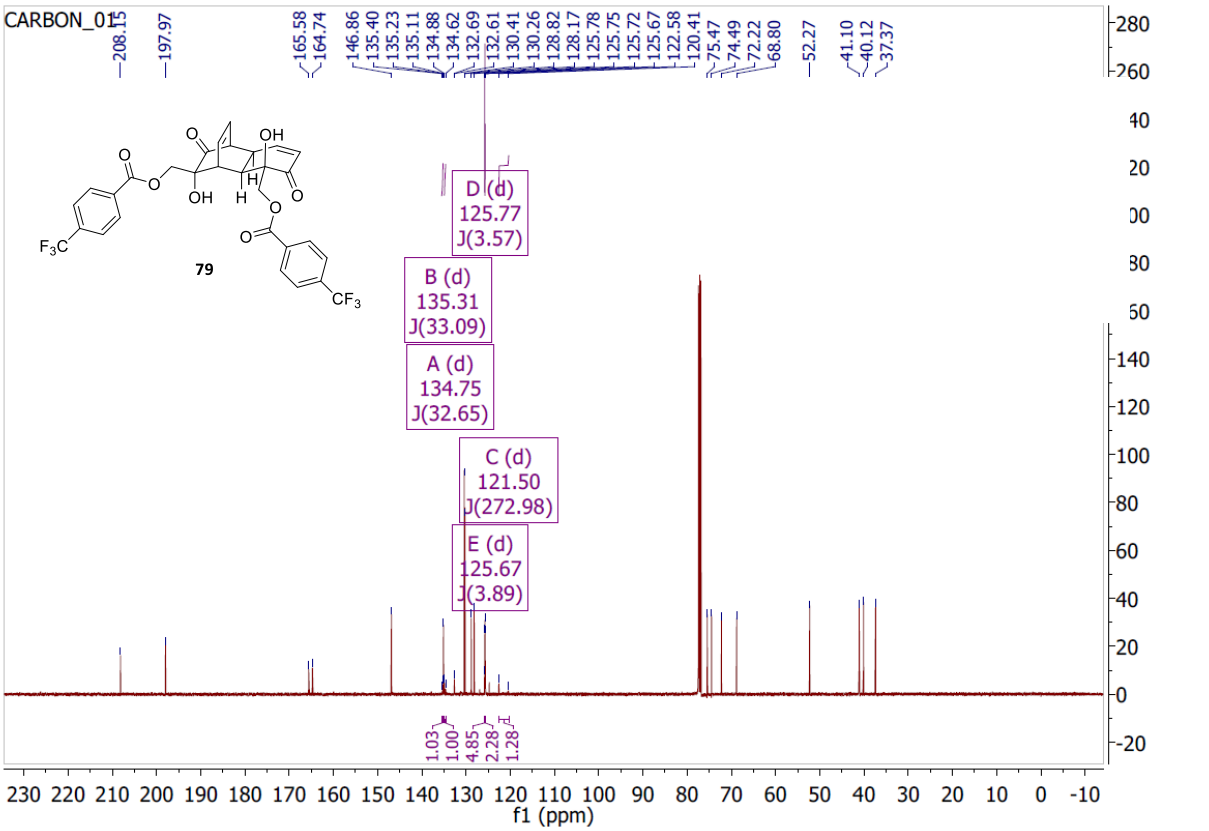
Acquisition Parameter

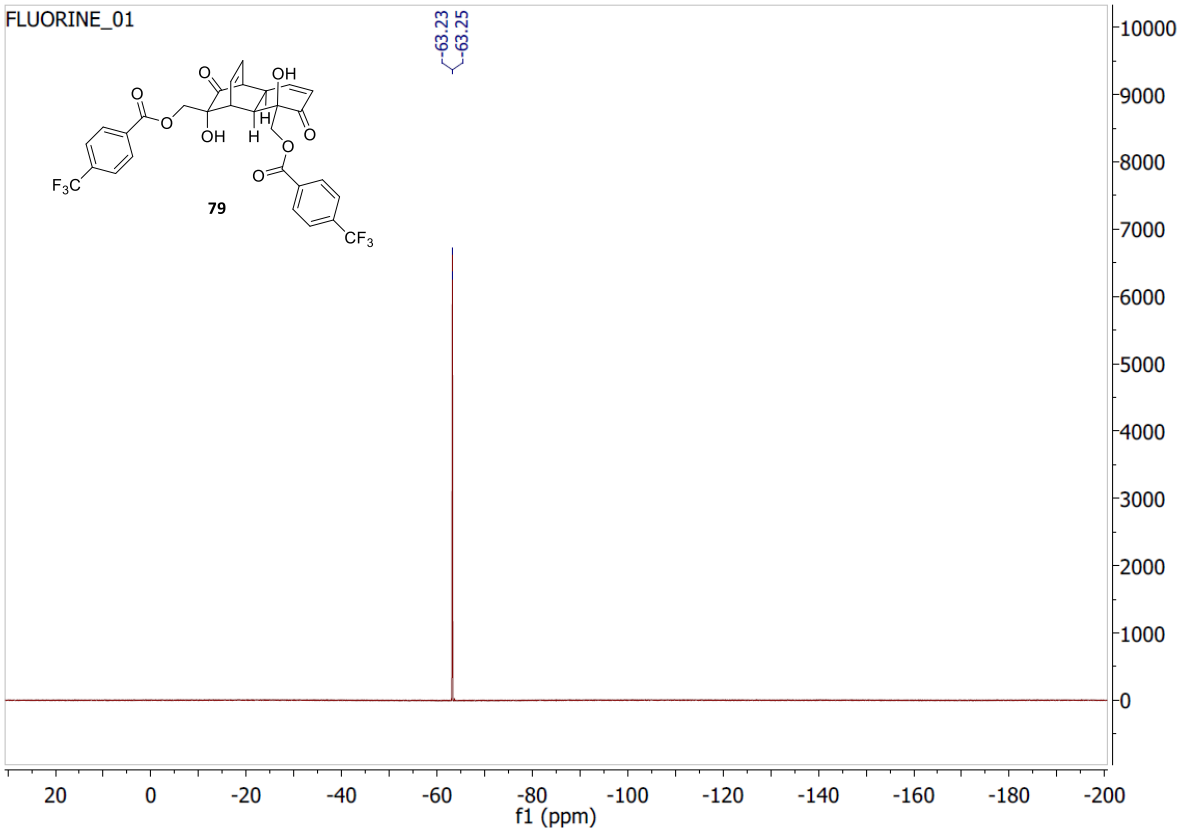
Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.5 Bar
Focus	Not active			Set Dry Heater	220 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	9.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

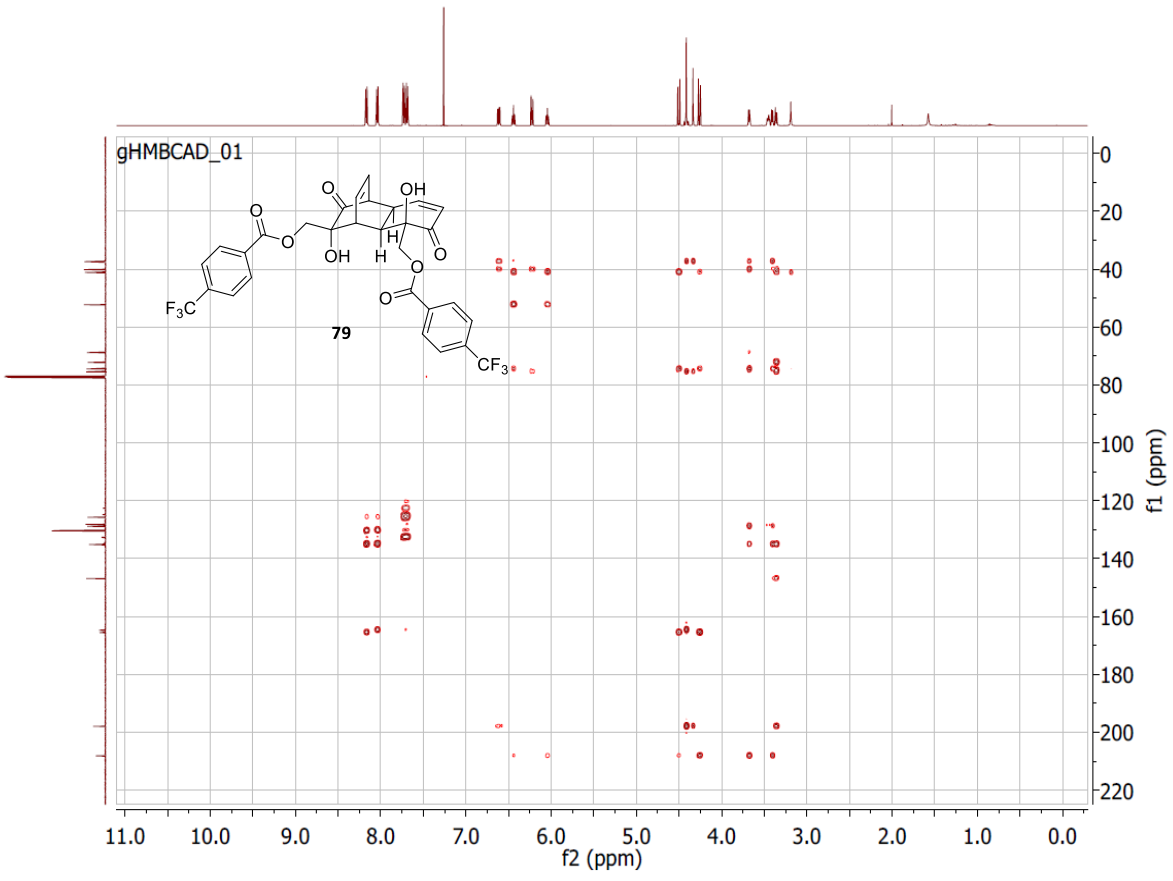


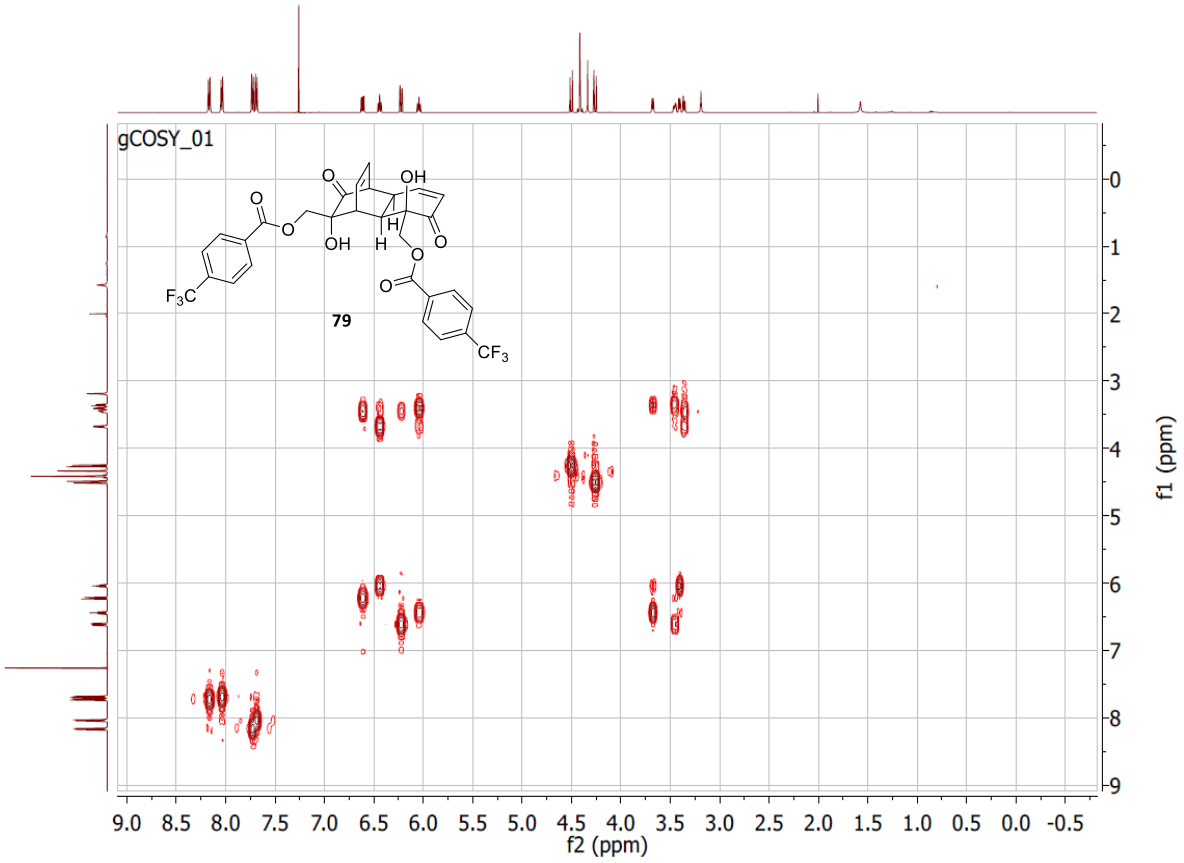
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
591.1240	1	C 30 H 21 F 6 O 6	100.00	591.1248	0.8	1.4	6.2	17.5	even	ok

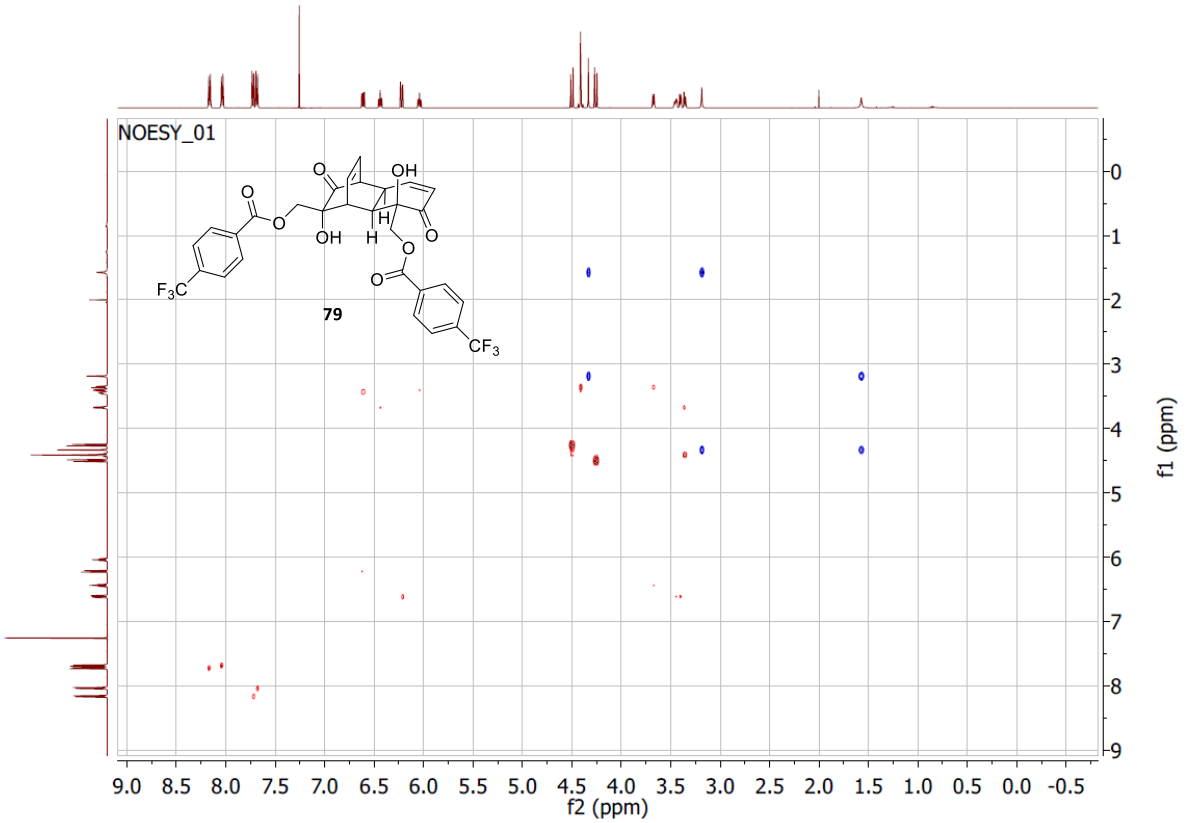

Q (d)
8.17
J(8.09)
O (d)
7.69
J(8.53)
N (d)
7.74
J(8.23)
P (d)
8.04
J(8.23)
M (dd)
6.61
J(10.12, 4.26)
K (dd)
6.22
J(10.11, 1.64)
J (ddd)
6.04
J(7.83, 6.05, 1.58)
L (ddd)
6.44
J(8.08, 6.65, 1.31)
H (d)
4.41
J(1.73)
G (s)
4.33
D (dd)
3.36
J(8.49, 2.16)
B (ddt)
3.45
J(8.31, 4.14, 1.82)
A (dt)
3.68
J(6.59, 1.88)
C (ddd)
3.41
J(6.07, 2.30, 1.30)
F (d)
4.26
J(11.89)
E (s)
3.15
I (d)
4.50
J(11.89)
79
1.86
1.86
1.90
1.89
1.04
0.95
0.93
0.92
0.98
1.93
0.82
0.97
1.00
0.96
1.00
0.99
0.84
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

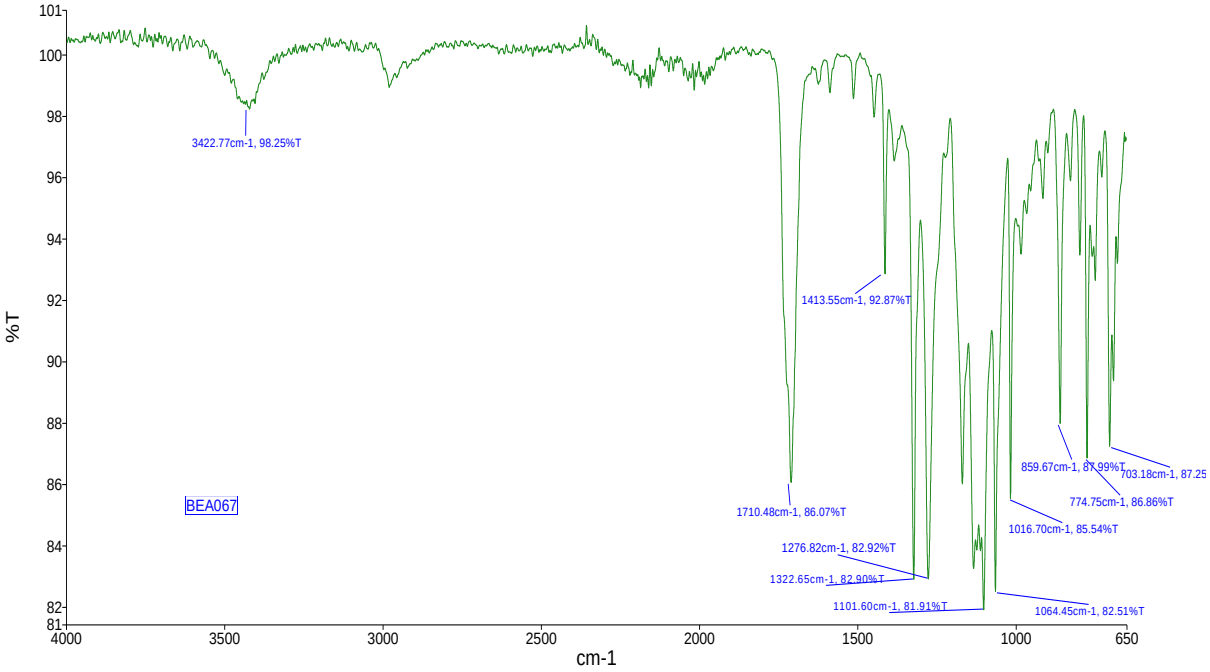

CARBON_01
208.15
197.97
165.58
164.74
146.86
135.40
135.23
135.11
134.88
134.62
132.69
132.61
130.41
130.26
128.82
128.17
125.78
125.75
125.72
125.67
122.58
120.41
75.47
74.49
72.22
68.80
52.27
41.10
40.12
37.37
D (d)
125.77
J(3.57)
B (d)
135.31
J(33.09)
A (d)
134.75
J(32.65)
C (d)
121.50
J(272.98)
E (d)
125.67
J(3.89)
79
1.03
1.00
4.85
2.28
1.28
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


FLUORINE_01
-63.23
-63.25
79
f1 (ppm)


gHMBCAD_01
79
f2 (ppm)
f1 (ppm)


gCOSY_01
OH
O
O
OH
H
O
O
F3C
79
O
O
CF3
f1 (ppm)
f2 (ppm)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
0 1 2 3 4 5 6 7 8 9


NOESY_01
OH
O
O
OH
H
O
O
F3C
79
O
O
CF3
f1 (ppm)
f2 (ppm)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
0 1 2 3 4 5 6 7 8 9



Confirmation of Expected Formula

_sel_I-BEA067

_sel_I-BEA067_345391_8_01_49940.d

nfirm Formula Positive 50to1500 loop inj.m

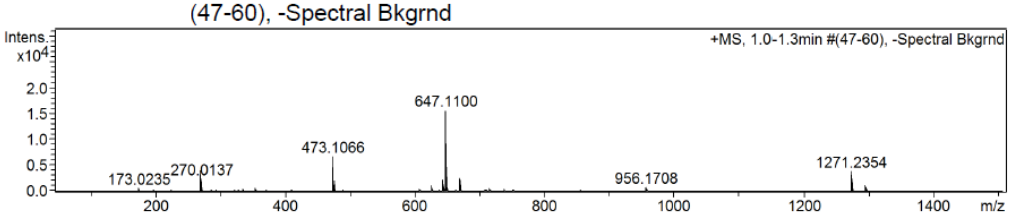
sitive electrospray (ESI)

Submitter Ben Alexander

Supervisor Simon Lewis

Acquisition Date 02/11/2015 15:23:48

(47-60), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	270.0137	2332	15.0	25	2460.1
2	473.1066	6690	42.9	176	8096.2
3	475.1073	2094	13.4	79	2509.9
4	625.1301	1196	7.7	167	481.9
5	642.1548	2286	14.7	343	698.9
6	647.1100	15581	100.0	2304	4451.3
7	648.1157	4750	30.5	736	1339.2
8	669.0920	2258	14.5	382	499.8
9	1271.2354	3814	24.5	846	2992.7
10	1272.2464	2396	15.4	548	1900.1

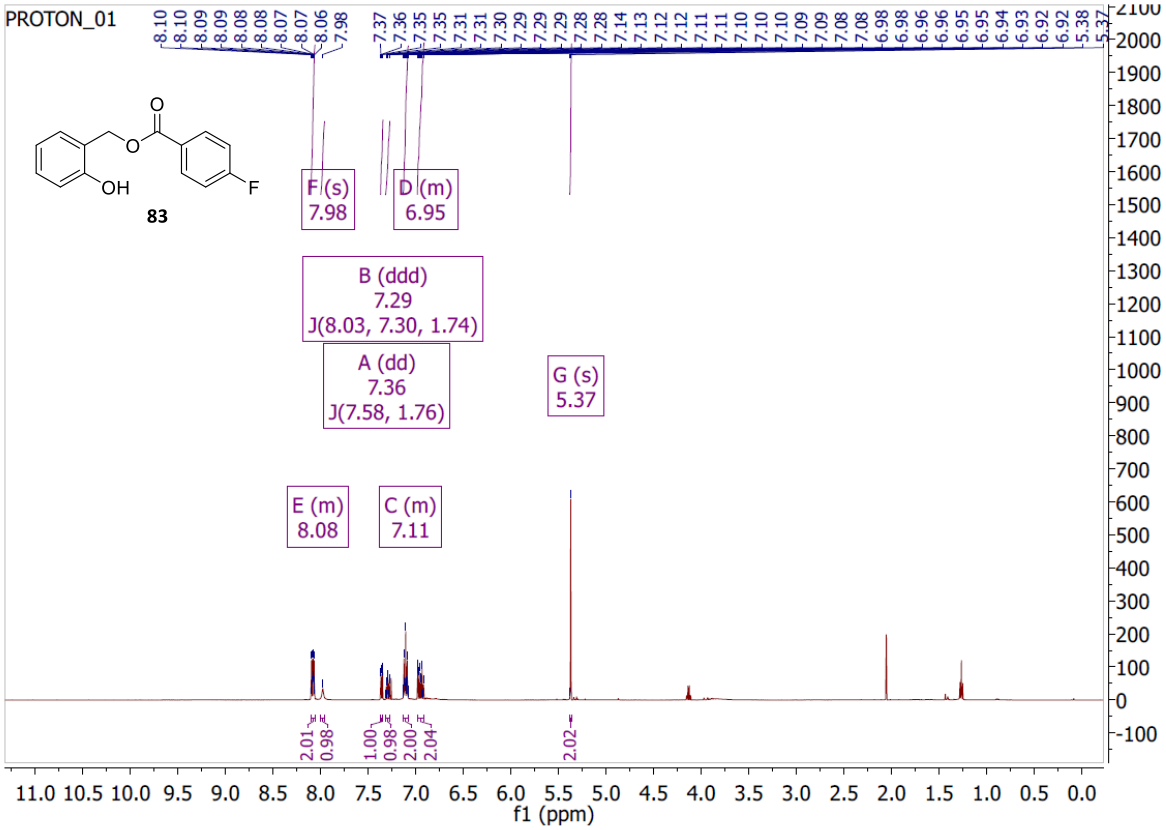
Generate Molecular Formula Parameters

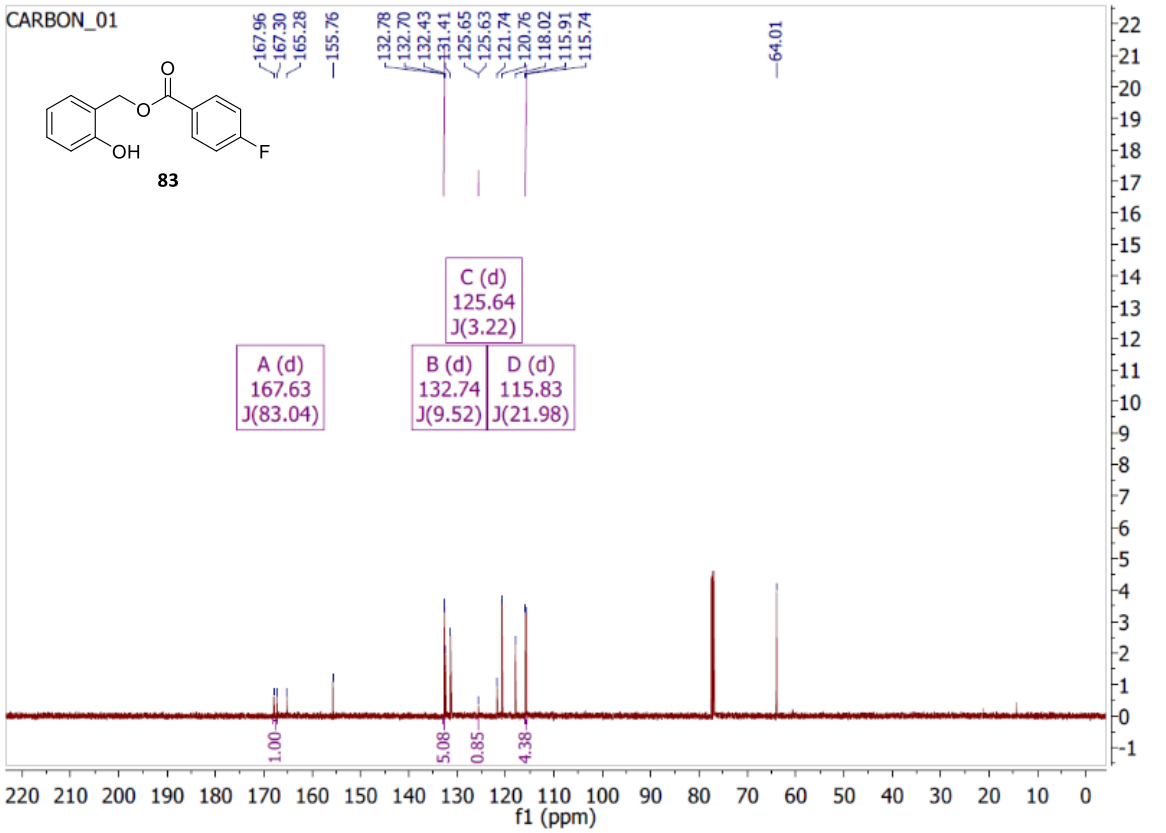
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

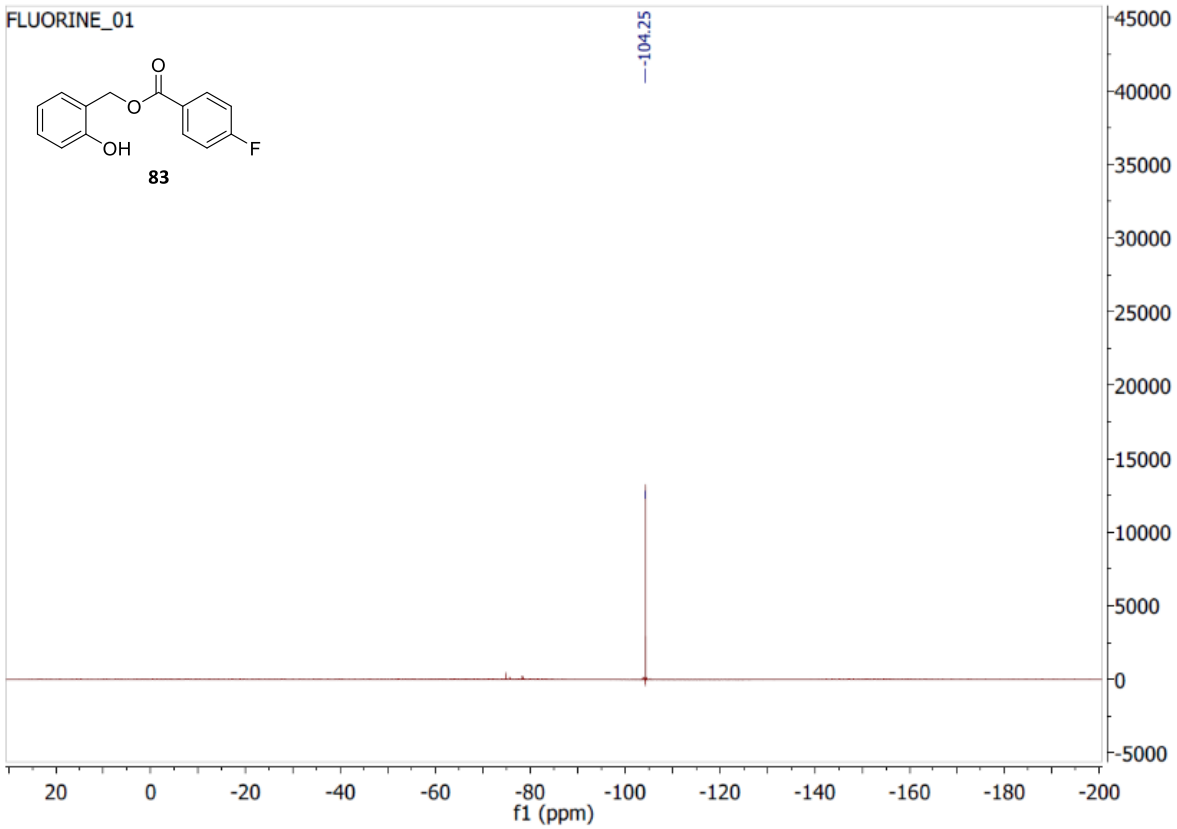
Expected Formula C30 H22 F6 O8 **Adduct(s):** H, Na

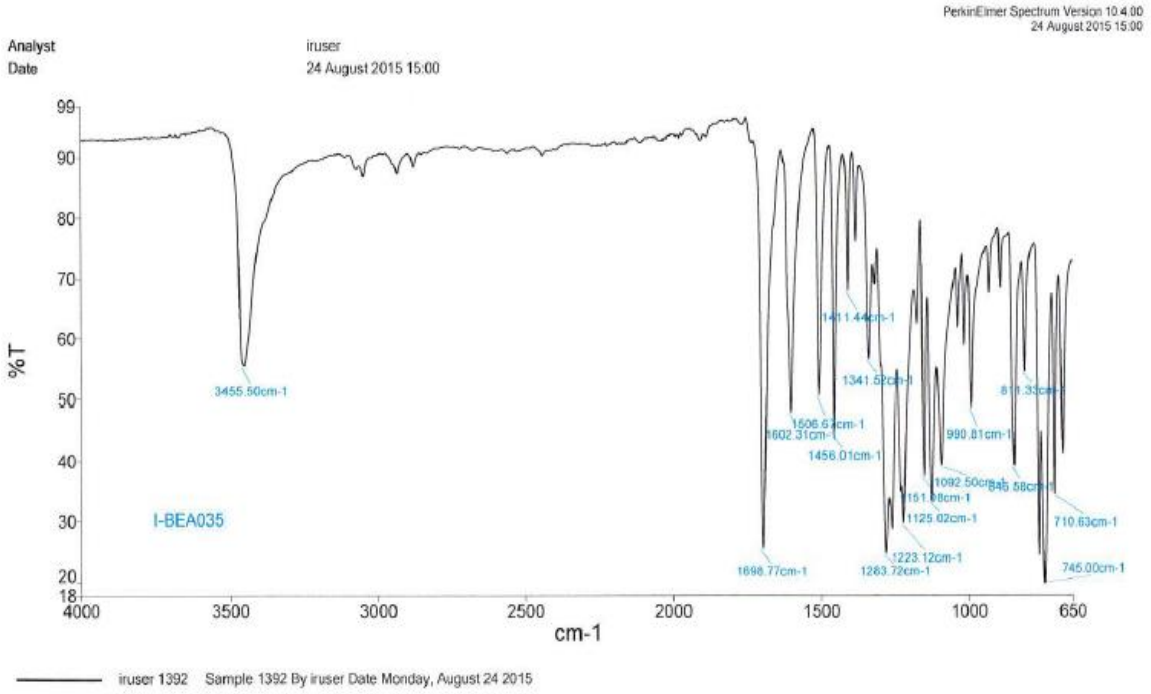
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	625.1301	625.129712	-1.50	0.0395	C 30 H 23 F 6 O 8
1	647.1100	647.111657	1.70	0.0163	C 30 H 22 F 6 Na 1 O 8

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication


PROTON_01
83
F (s)
7.98
D (m)
6.95
B (ddd)
7.29
J(8.03, 7.30, 1.74)
A (dd)
7.36
J(7.58, 1.76)
G (s)
5.37
E (m)
8.08
C (m)
7.11
f1 (ppm)


CARBON_01
83
C (d)
125.64
J(3.22)
A (d)
167.63
J(83.04)
B (d)
132.74
J(9.52)
D (d)
115.83
J(21.98)
f1 (ppm)

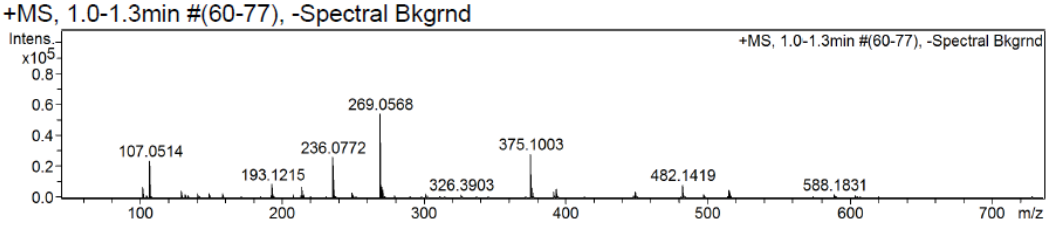

FLUORINE_01
-104.25
O
O
OH
F
83
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)


PerkinElmer Spectrum Version 10.4.00
24 August 2015 15:00
Analyst
iruser
Date
24 August 2015 15:00
%T
99
90
80
70
60
50
40
30
20
18
3455.50cm-1
1602.31cm-1
1456.01cm-1
1341.52cm-1
990.81cm-1
1092.50cm-1
1125.02cm-1
710.63cm-1
1698.77cm-1
1223.12cm-1
1283.72cm-1
745.00cm-1
I-BEA035
4000
3500
3000
2500
2000
1500
1000
650
cm-1
iruser 1392 Sample 1392 By iruser Date Monday, August 24 2015

Confirmation of Expected Formula

Sample-ID	ba_sel_I-BEA035 B	Submitter	Ben Alexander
Analysis Name	ba_sel_I-BEA035 B_343957_14_01_48377.d	Supervisor	Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	04/06/2015 12:15:27
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	102.1279	6896	12.8	94	3793.2
2	107.0514	23911	44.5	543	11537.7
3	193.1215	8785	16.3	143	1361.9
4	214.1059	6836	12.7	155	727.9
5	236.0772	26091	48.5	474	2001.4
6	269.0568	53753	100.0	2917	4606.8
7	270.0627	7276	13.5	392	636.4
8	375.1003	28246	52.5	2290	3259.4
9	393.2996	5765	10.7	455	539.6
10	482.1419	8281	15.4	799	1107.9

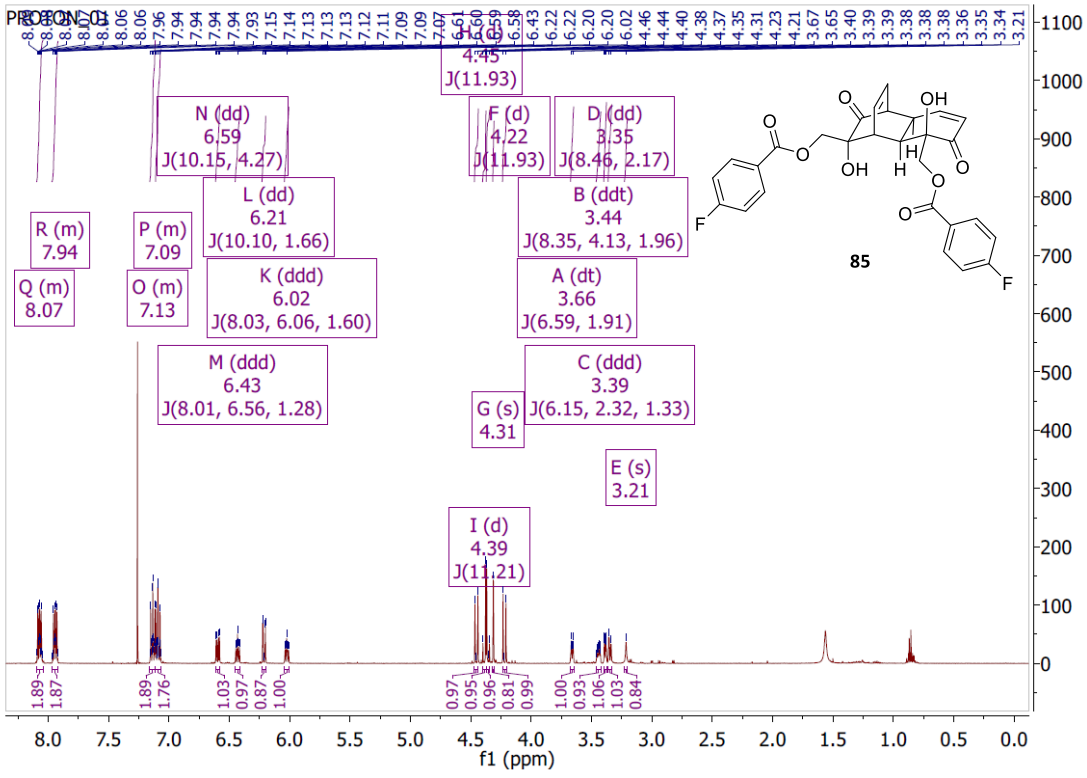
Generate Molecular Formula Parameters

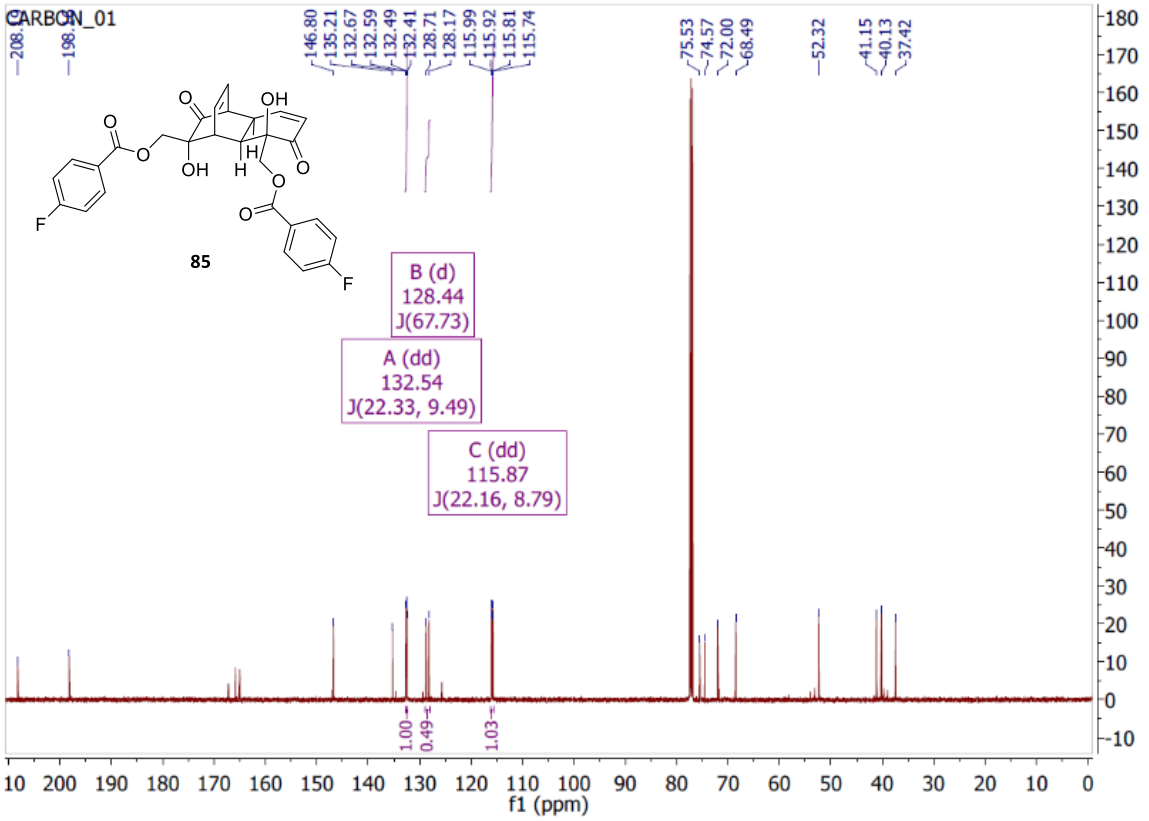
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

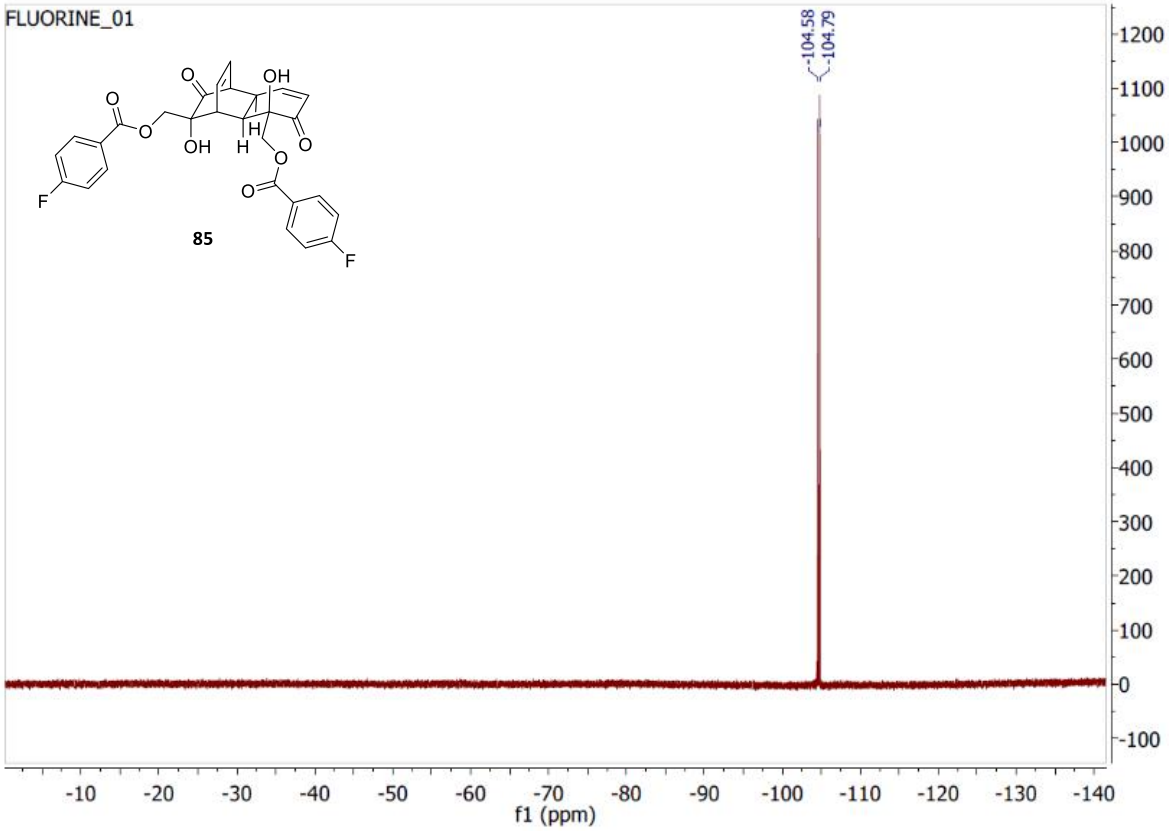
Expected Formula C14 H11 F1 O3 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	269.0568	269.058992	6.20	0.0134	C 14 H 11 F 1 Na 1 O 3

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication




CARBON_01
208.
198.
146.80
135.21
132.67
132.59
132.49
132.41
128.71
128.17
115.99
115.92
115.81
115.74
75.53
74.57
72.00
68.49
52.32
41.15
40.13
37.42
85
B (d)
128.44
J(67.73)
A (dd)
132.54
J(22.33, 9.49)
C (dd)
115.87
J(22.16, 8.79)
1.00
0.49
1.03
f1 (ppm)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-104.79
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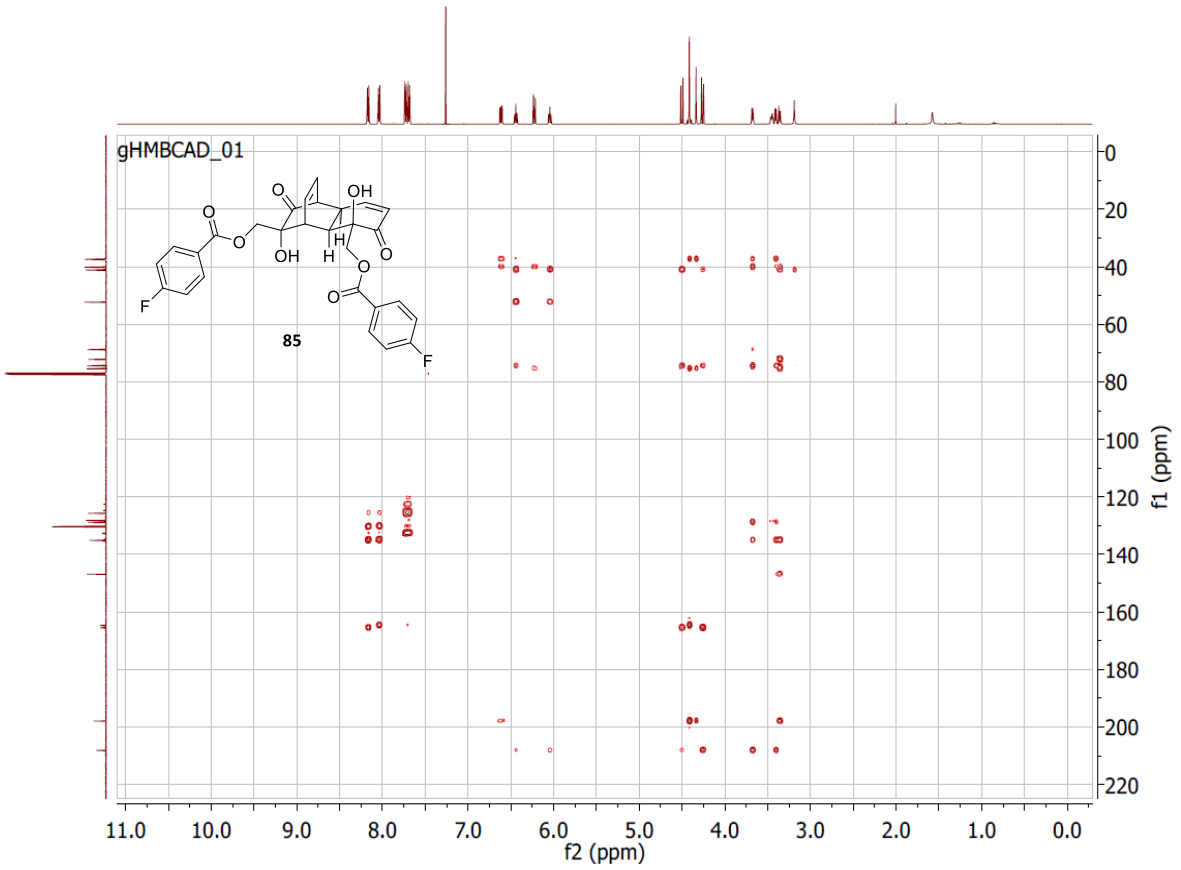
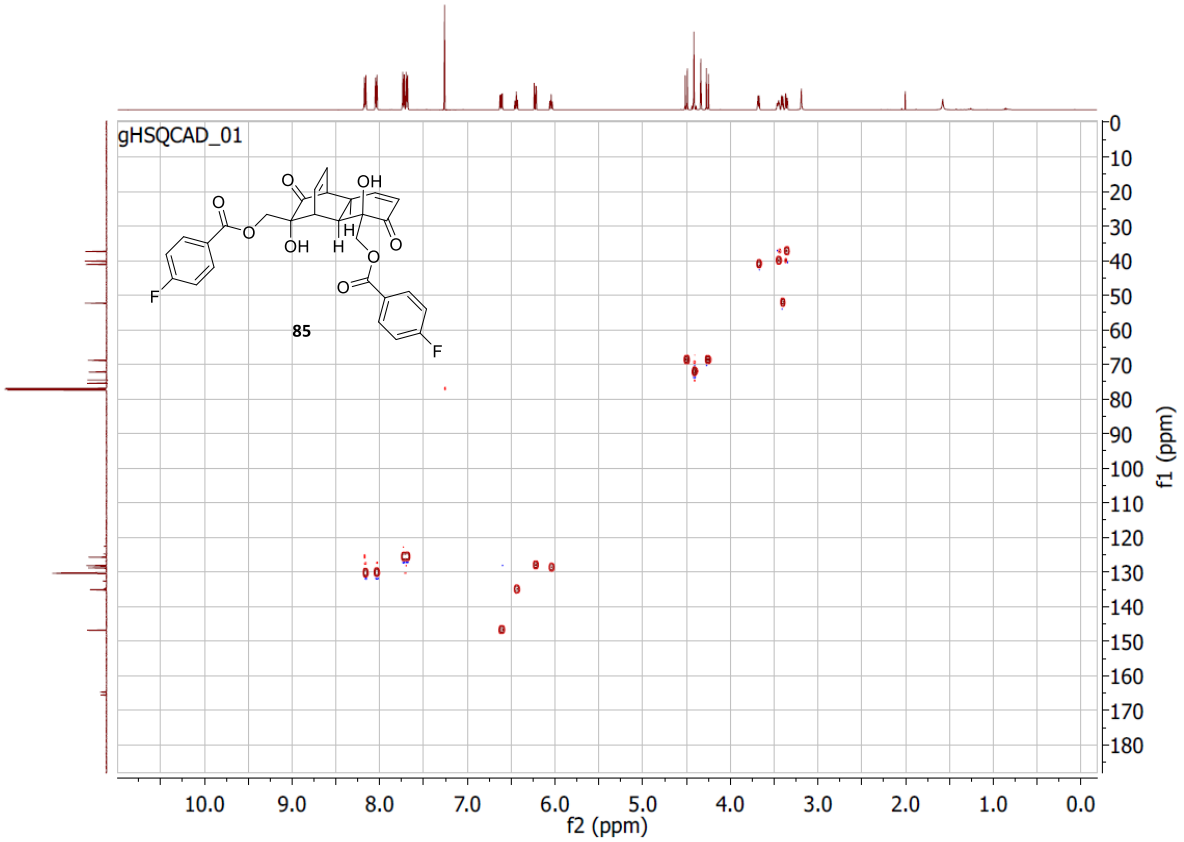
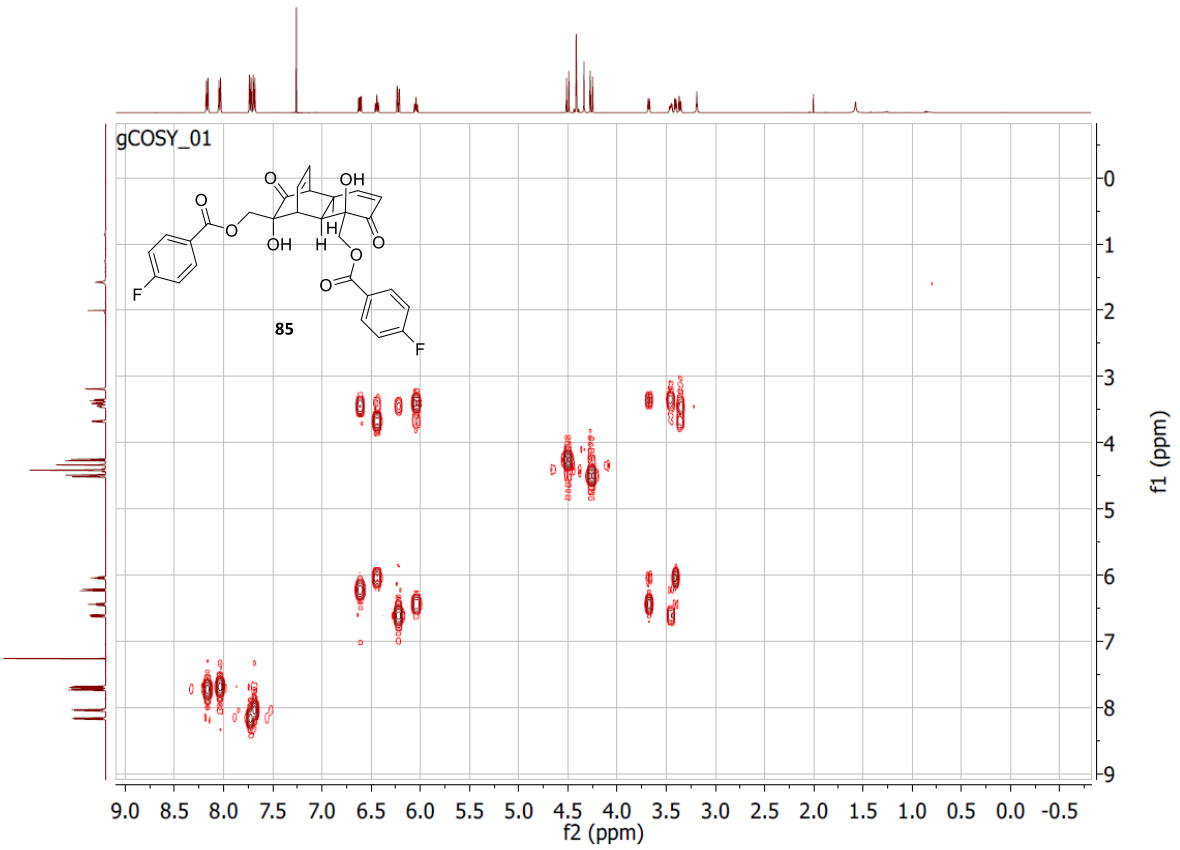
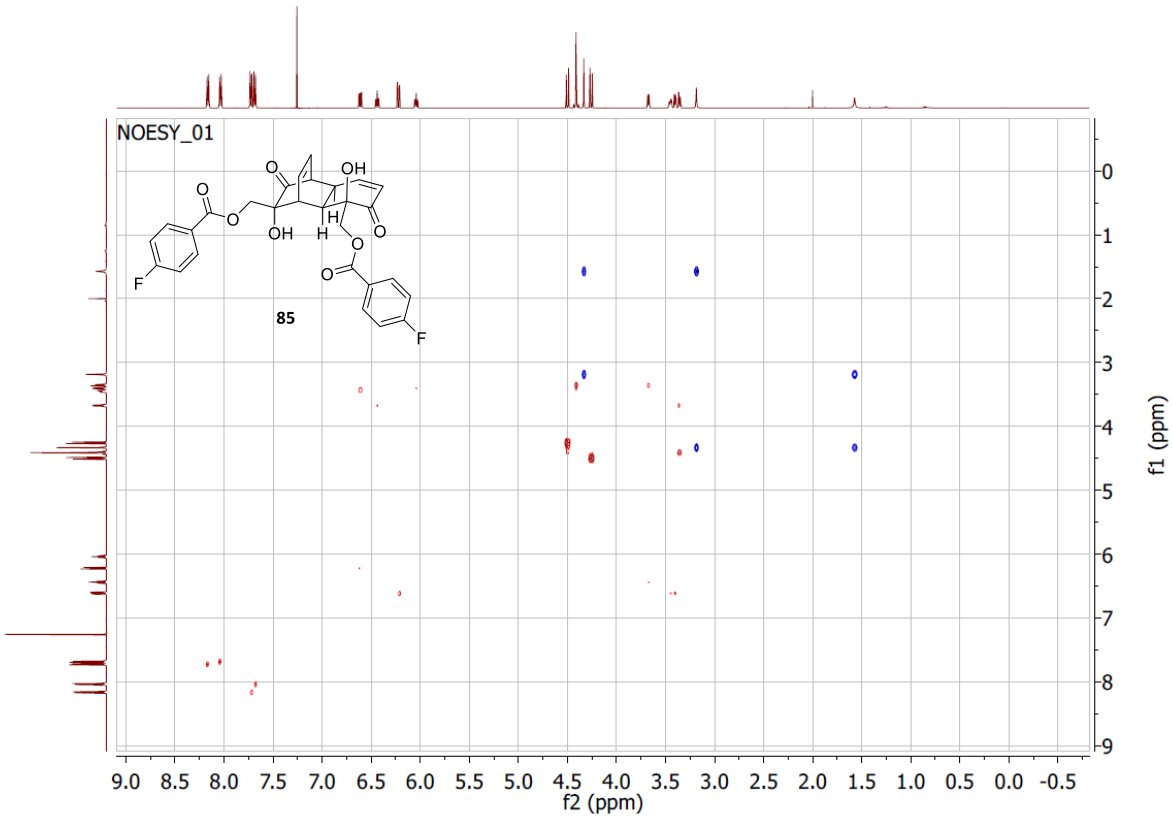
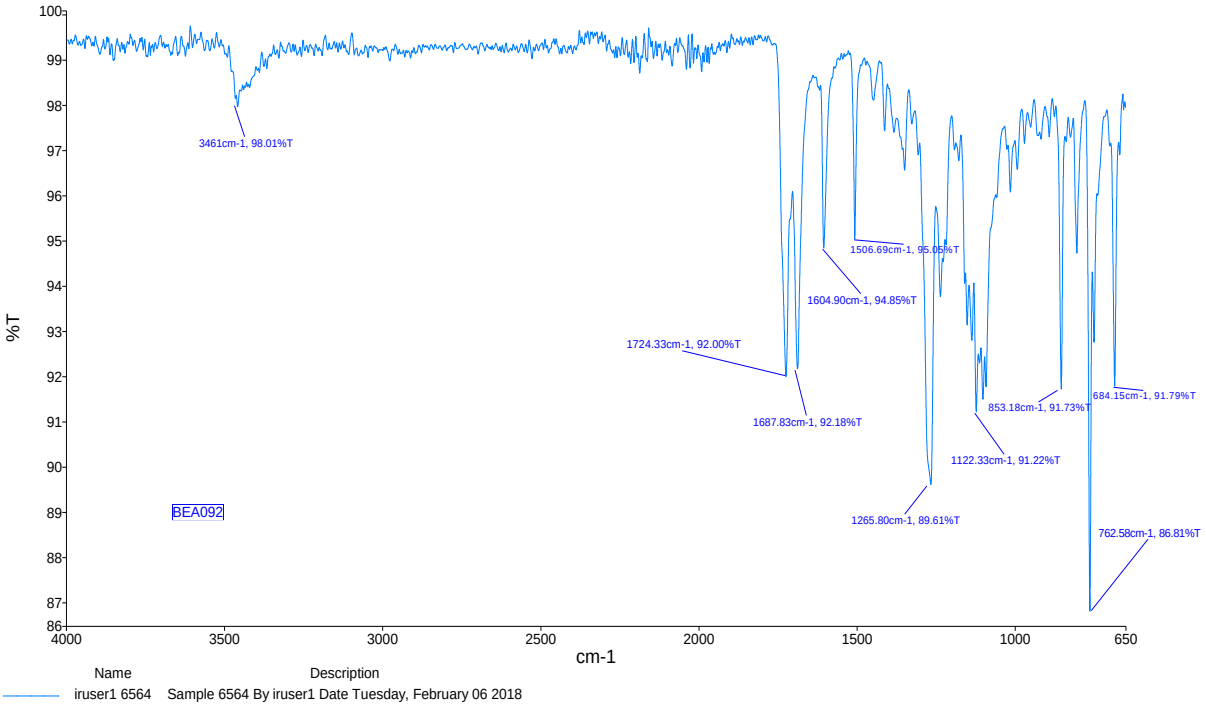
f1 (ppm)


gHMBCAD_01
85
f2 (ppm)
f1 (ppm)


gHSQCAD_01
85
f2 (ppm)
f1 (ppm)


gCOSY_01
85
f2 (ppm)
f1 (ppm)

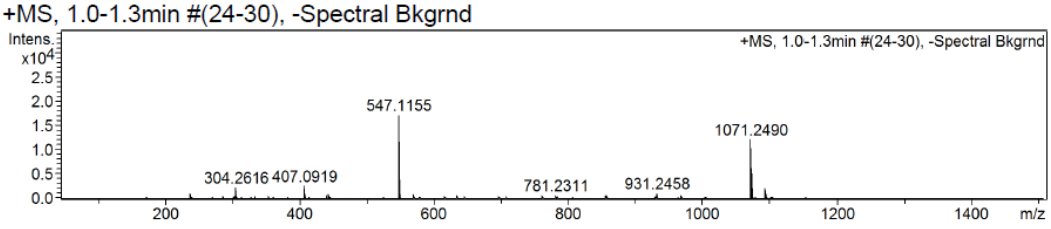

NOESY_01
85
f2 (ppm)
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_I-BEA092	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_I-BEA092_347654_27_01_52427.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to1500 loop inj.m	Acquisition Date	10/05/2016 16:34:21
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(24-30), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	304.2616	2263	13.2	147	2710.9
2	407.0919	2556	14.9	213	2420.7
3	547.1155	17195	100.0	1950	2282.7
4	548.1201	4632	26.9	555	607.1
5	931.2458	1109	6.5	116	157.9
6	1071.2490	12062	70.1	2561	1806.2
7	1072.2489	6270	36.5	999	947.6
8	1073.2541	1815	10.6	368	276.8
9	1093.2356	2116	12.3	341	396.3
10	1094.2422	1086	6.3	192	205.7

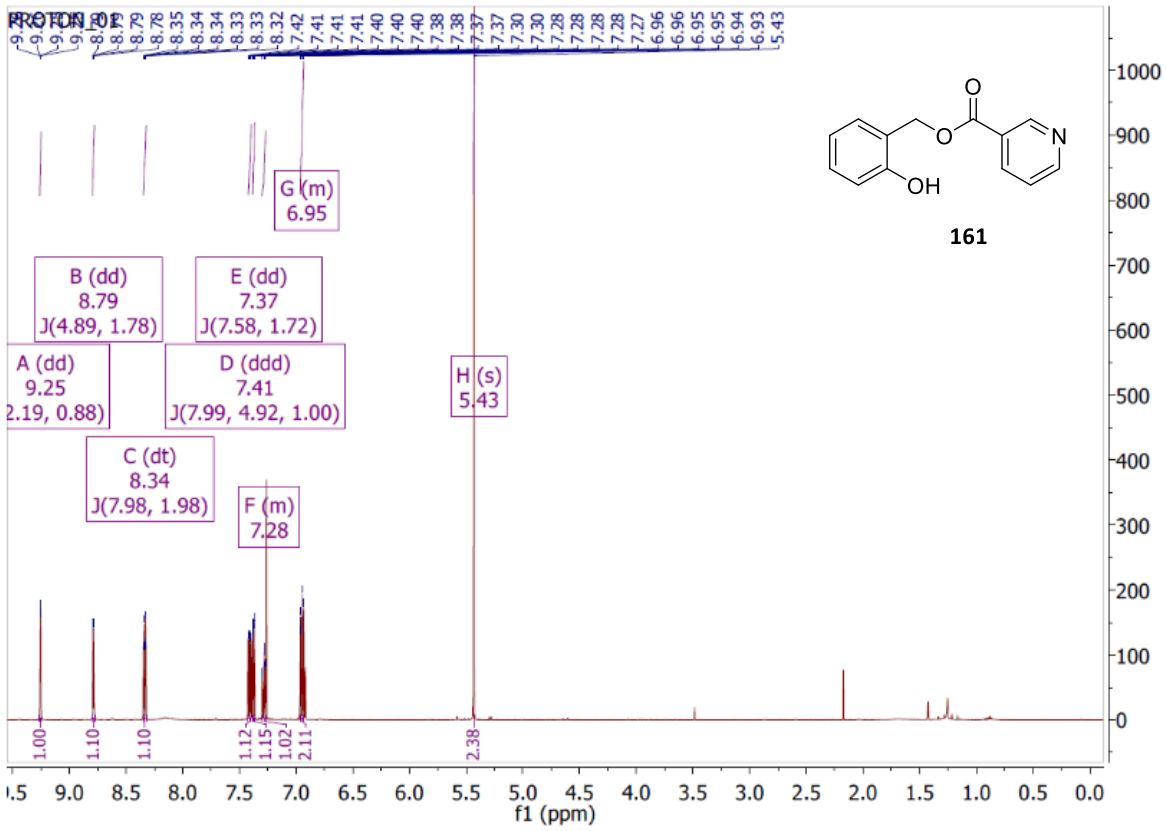
Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

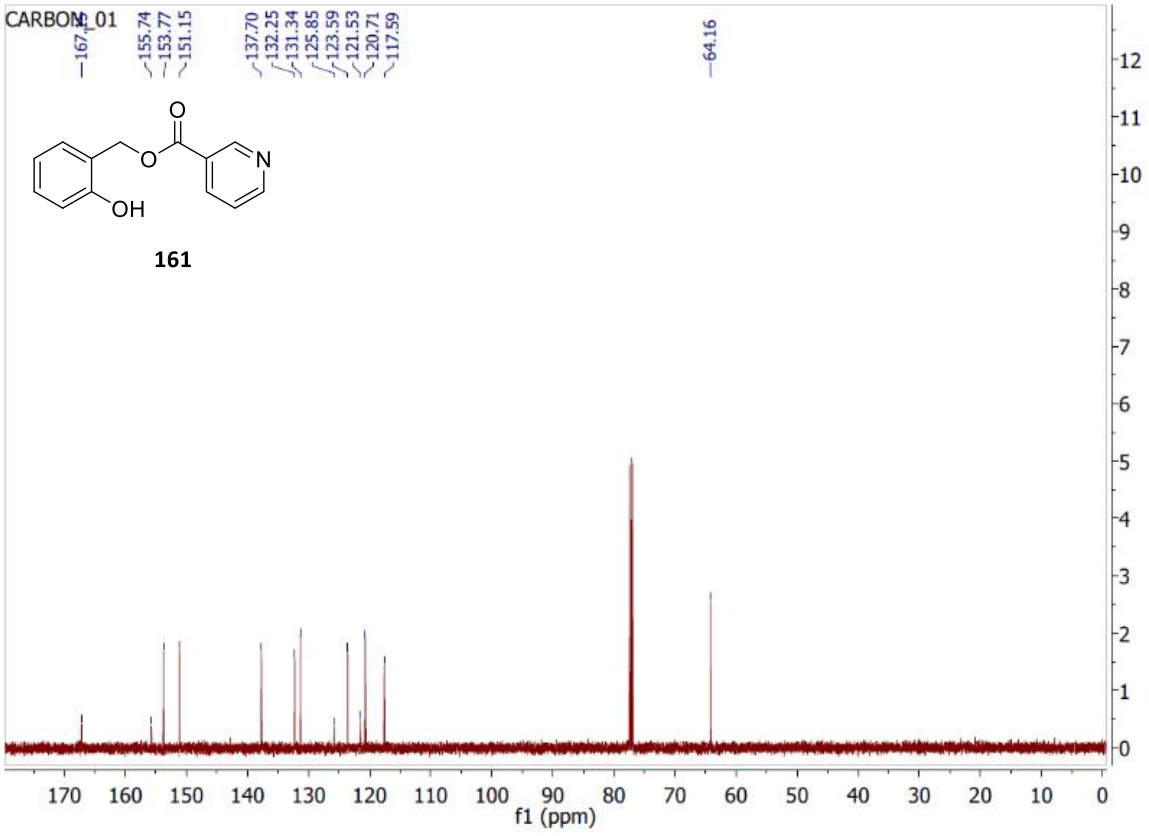
Expected Formula C28 H22 F2 O8 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	547.1155	547.118044	3.60	0.0174	C 28 H 22 F 2 Na 1 O 8

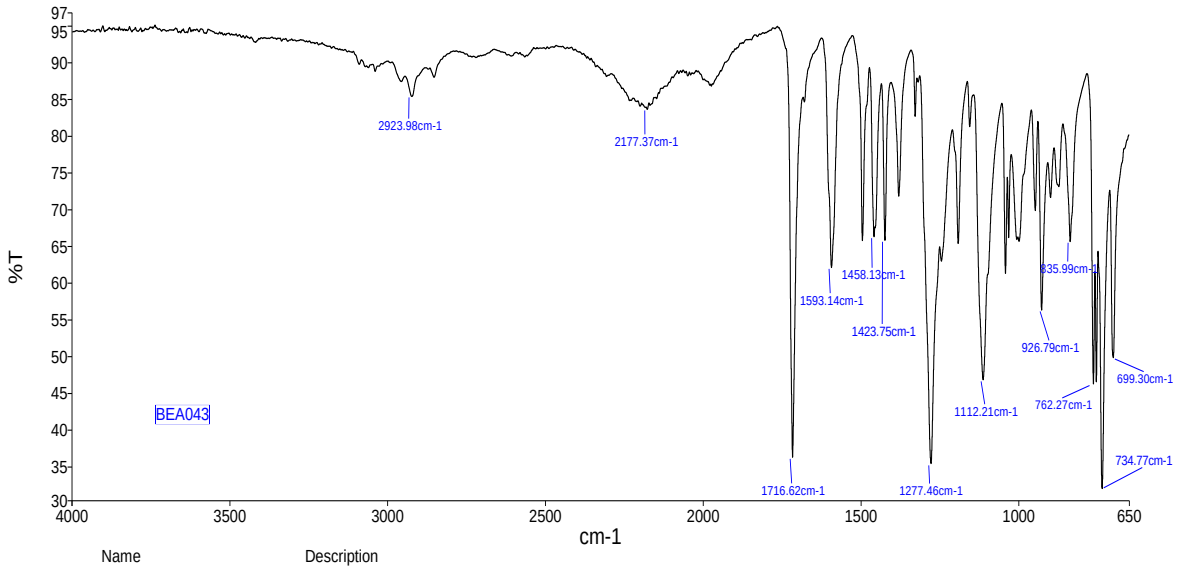
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication


PROTON_01
G (m)
6.95
B (dd)
8.79
J(4.89, 1.78)
E (dd)
7.37
J(7.58, 1.72)
A (dd)
9.25
2.19, 0.88)
D (ddd)
7.41
J(7.99, 4.92, 1.00)
H (s)
5.43
C (dt)
8.34
J(7.98, 1.98)
F (m)
7.28
1.00
1.10
1.10
1.12
1.15
1.02
2.11
2.38
f1 (ppm)

161


CARBON_01
167.41
155.74
153.77
151.15
137.70
132.25
131.34
125.85
123.59
121.53
120.71
117.59
64.16
f1 (ppm)

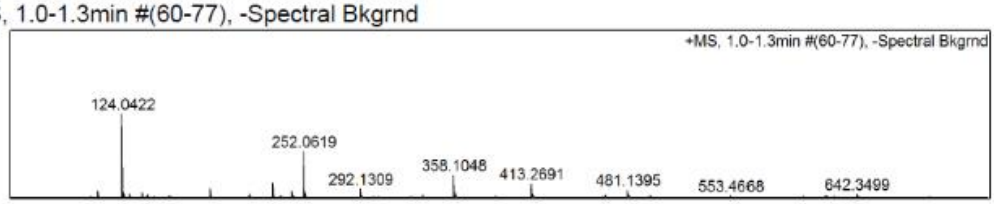
161



Confirmation of Expected Formula

Sample-ID	ba_sel_I-BEA043	Submitter	Ben Alexander
Analysis Name	ba_sel_I-BEA043_344124_70_01_48553.d	Supervisor	Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	22/06/2015 11:43:13
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	107.0513	15133	8.4	332	2074.9
2	124.0422	180287	100.0	3933	23877.6
3	186.0921	18913	10.5	715	4003.1
4	230.0795	32661	18.1	1504	2543.0
5	244.0951	15535	8.6	746	900.6
6	252.0619	99429	55.2	4600	5047.8
7	292.1309	19061	10.6	1106	1586.7
8	358.1048	49023	27.2	3406	3574.1
9	413.2691	30029	16.7	2504	2238.5
10	481.1395	16750	9.3	1804	658.4

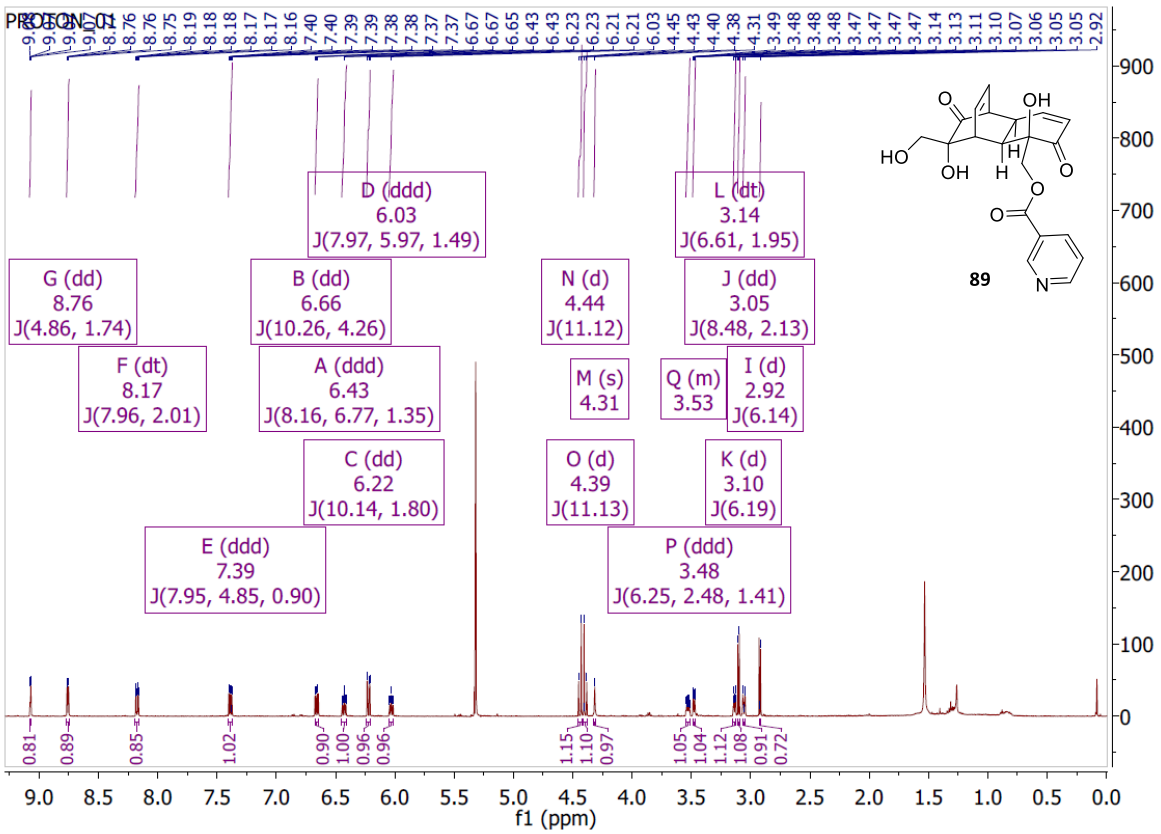
Generate Molecular Formula Parameters

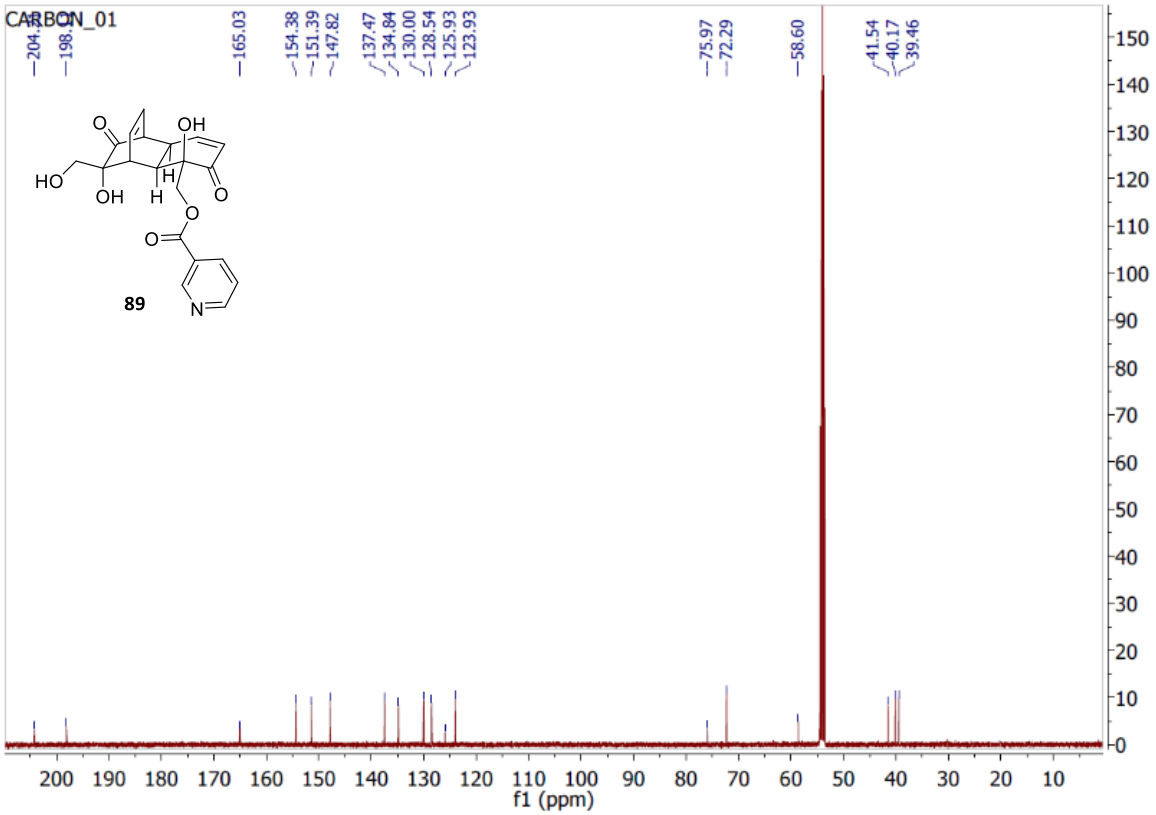
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

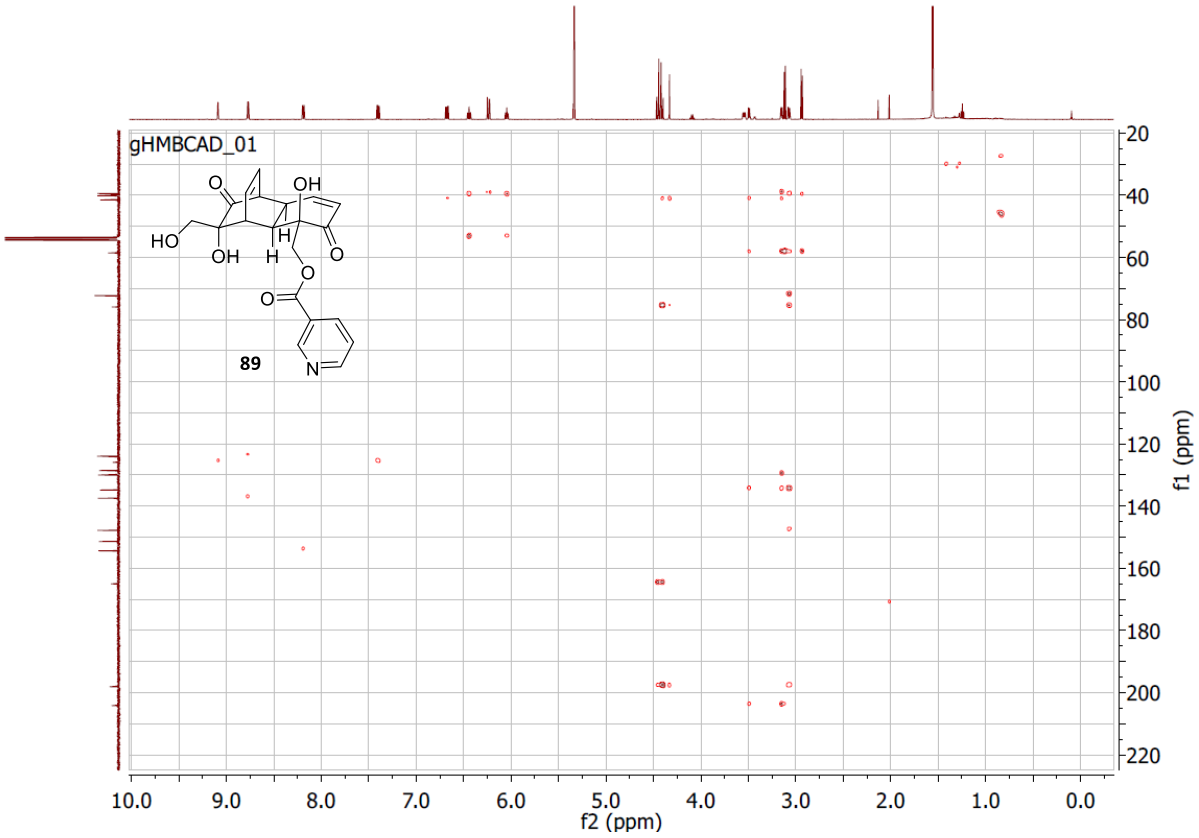
Expected Formula C13 H11 N1 O3 **Adduct(s):** H, Na

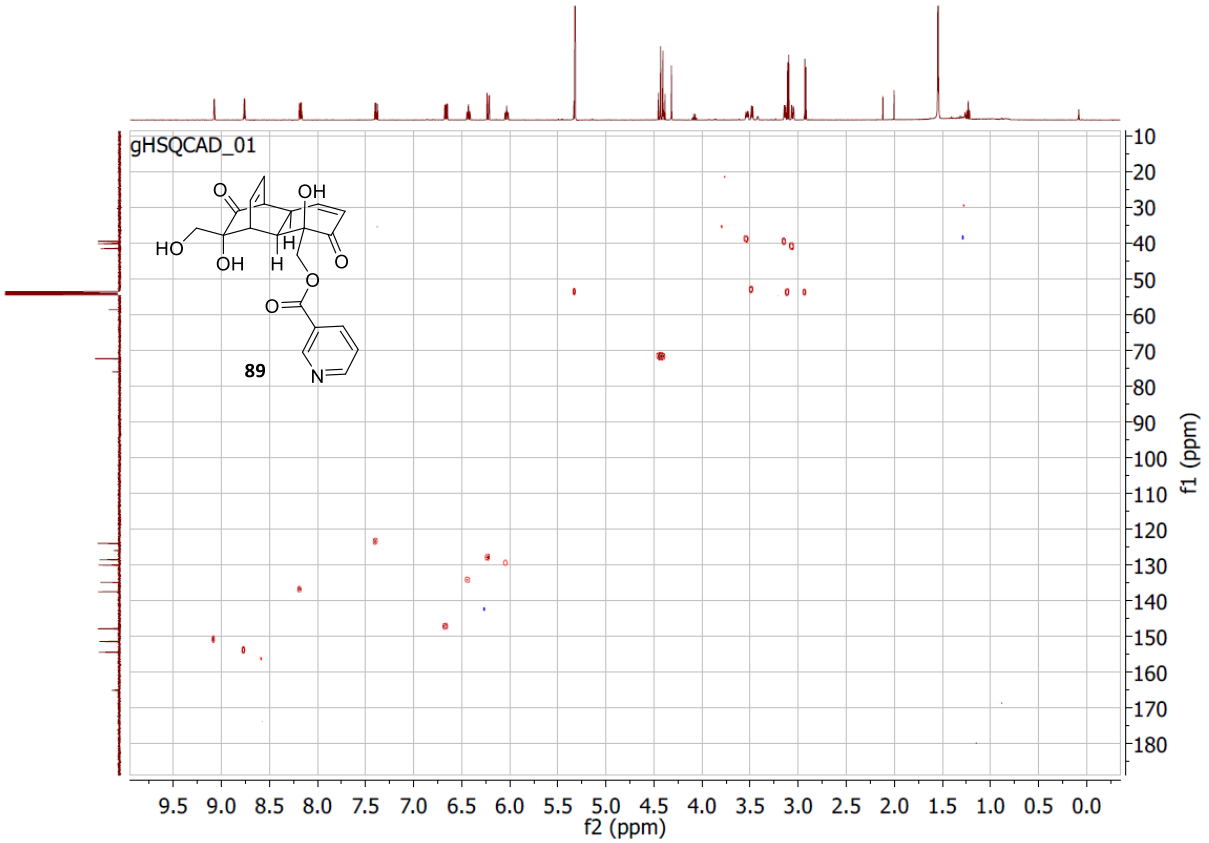
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	230.0795	230.081718	7.40	0.0472	C 13 H 12 N 1 O 3
1	252.0619	252.063663	5.00	0.0031	C 13 H 11 N 1 Na 1 O 3

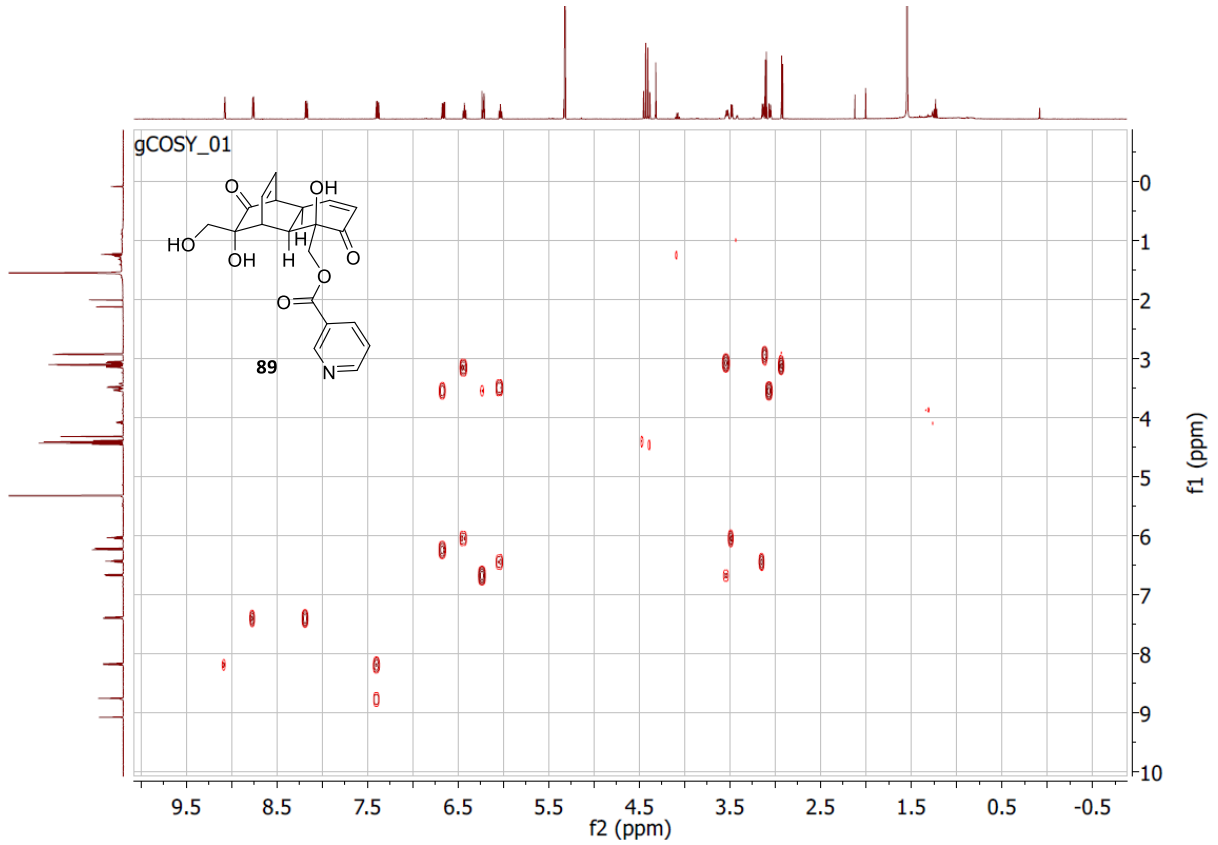
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

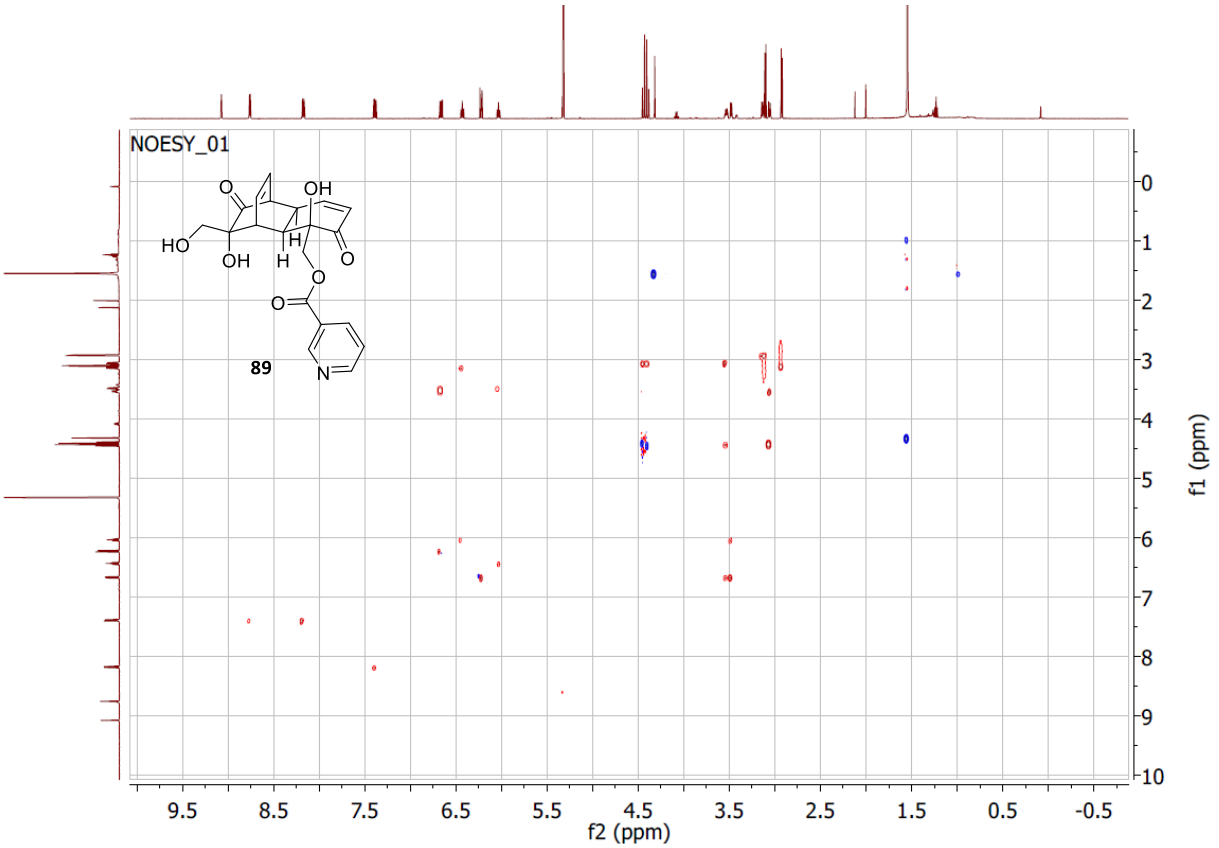

PROTON_01
G (dd)
8.76
J(4.86, 1.74)
F (dt)
8.17
J(7.96, 2.01)
D (ddd)
6.03
J(7.97, 5.97, 1.49)
B (dd)
6.66
J(10.26, 4.26)
A (ddd)
6.43
J(8.16, 6.77, 1.35)
C (dd)
6.22
J(10.14, 1.80)
E (ddd)
7.39
J(7.95, 4.85, 0.90)
N (d)
4.44
J(11.12)
M (s)
4.31
O (d)
4.39
J(11.13)
L (dt)
3.14
J(6.61, 1.95)
J (dd)
3.05
J(8.48, 2.13)
Q (m)
3.53
I (d)
2.92
J(6.14)
K (d)
3.10
J(6.19)
P (ddd)
3.48
J(6.25, 2.48, 1.41)
89
f1 (ppm)

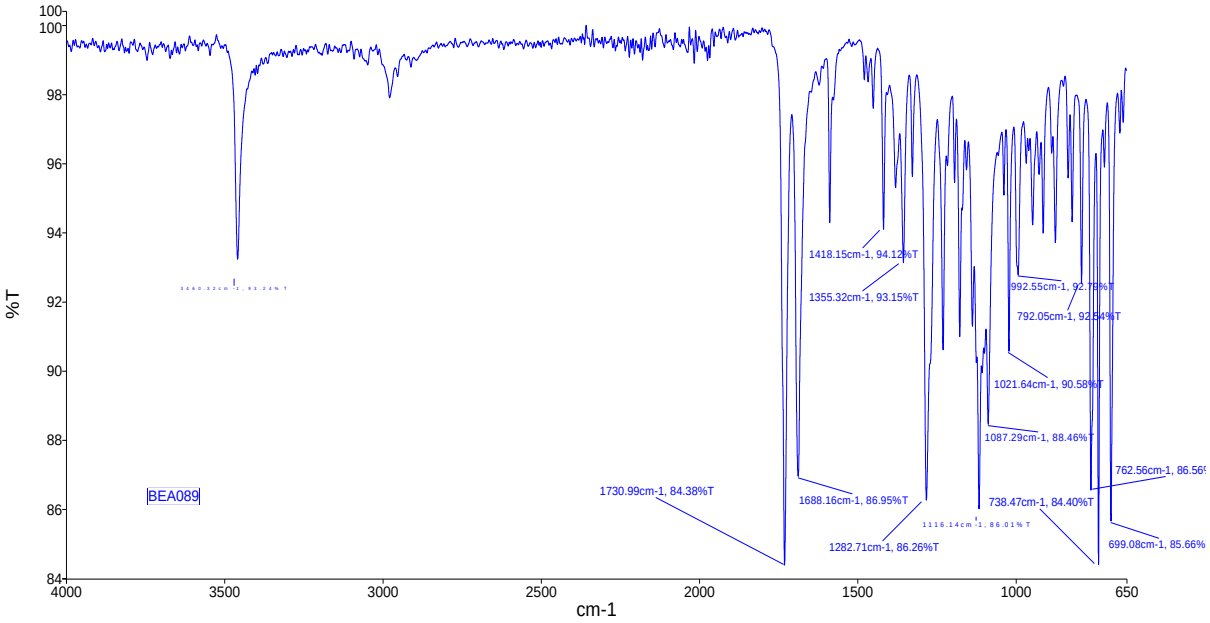

CARBON_01
89
f1 (ppm)


gHMBCAD_01
89
f2 (ppm)
f1 (ppm)


gHSQCAD_01
89
f2 (ppm)
f1 (ppm)


gCOSY_01
89
f2 (ppm)
f1 (ppm)


NOESY_01
89
f2 (ppm)
f1 (ppm)



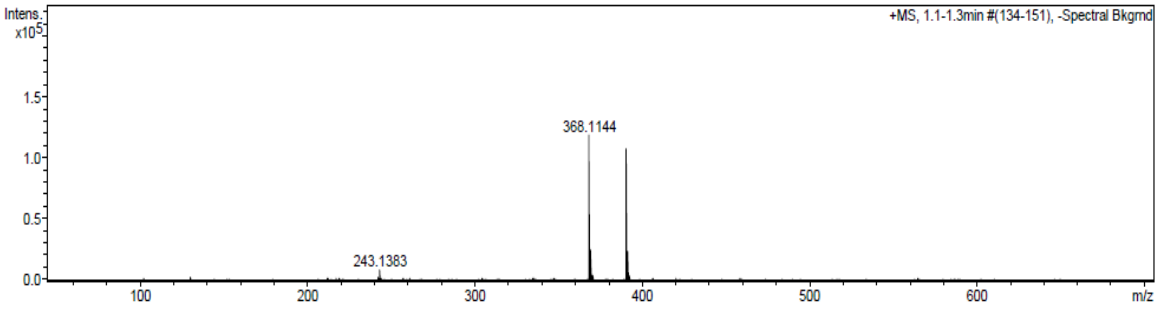
Mass Spectrum SmartFormula Report

Analysis Info

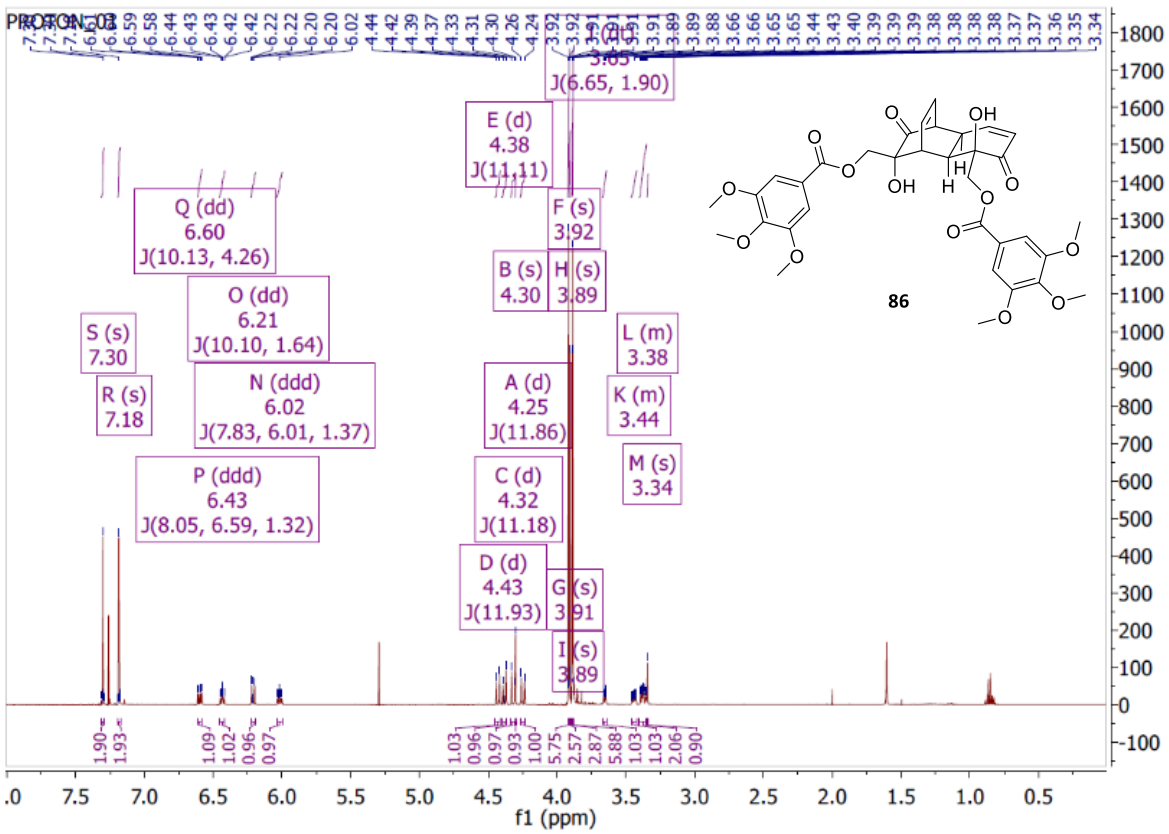
Analysis Name	Z:\ba_sel_BEA089_358361_42_01_64739.d	Acquisition Date	8/14/2018 11:22:07 AM
Method	Confirm Formula Positive 50to500 loop inj.m	Operator	admin
Sample Name	ba_sel_BEA089_358361	Instrument / Ser#	micrOTOF 161
Comment			

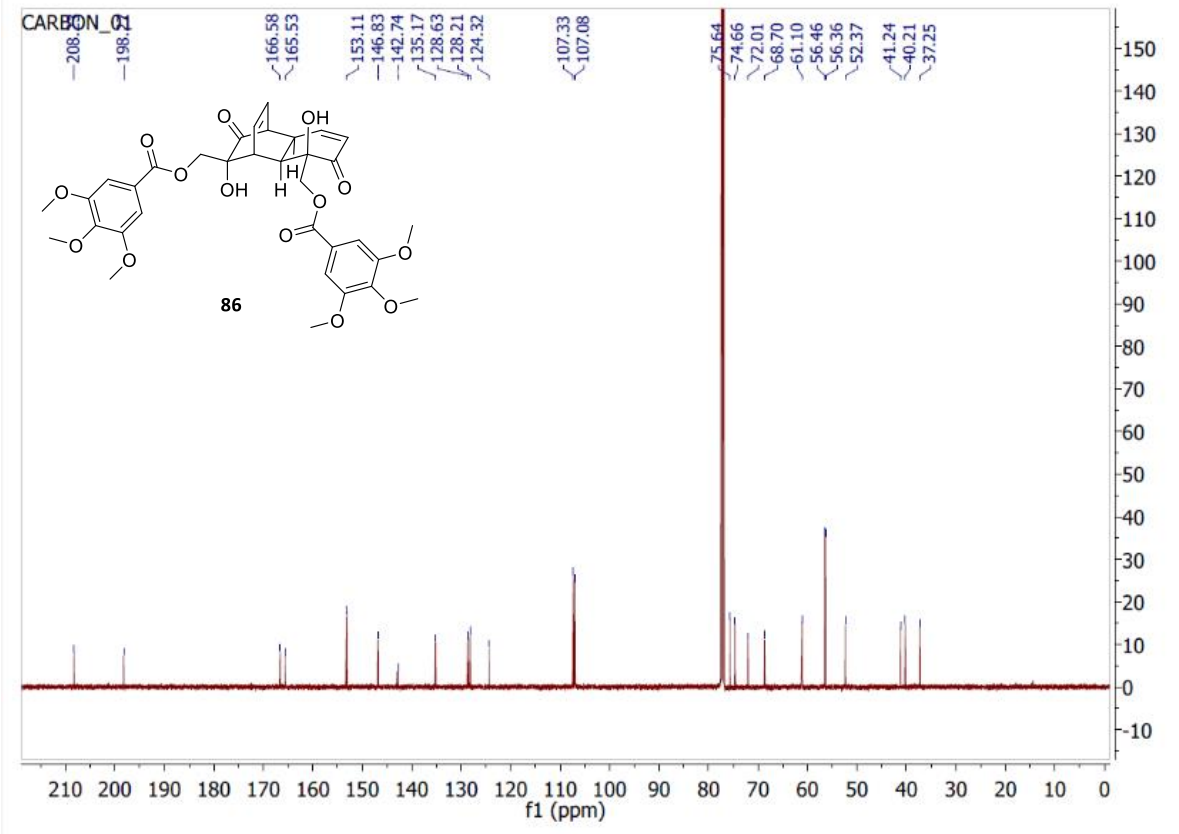
Acquisition Parameter

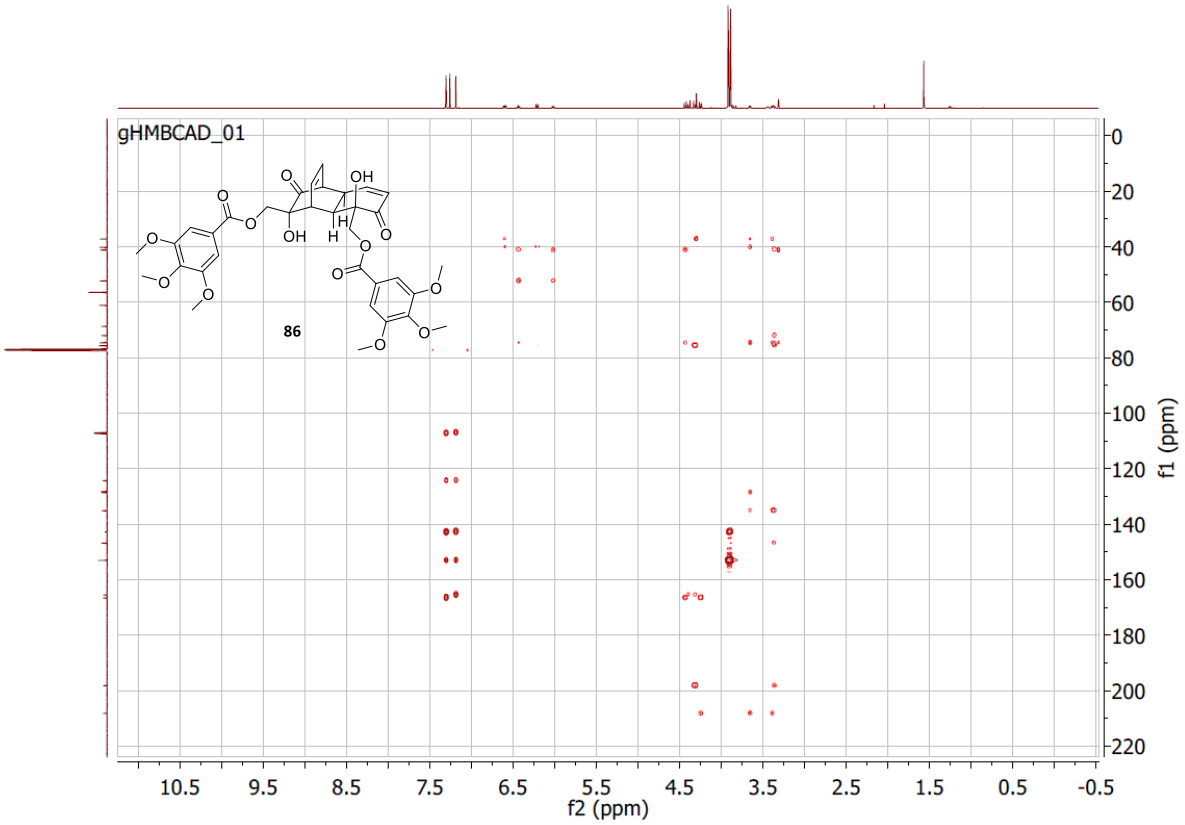
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.2 Bar
Focus	Not active			Set Dry Heater	220 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.2 l/min
Scan End	700 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

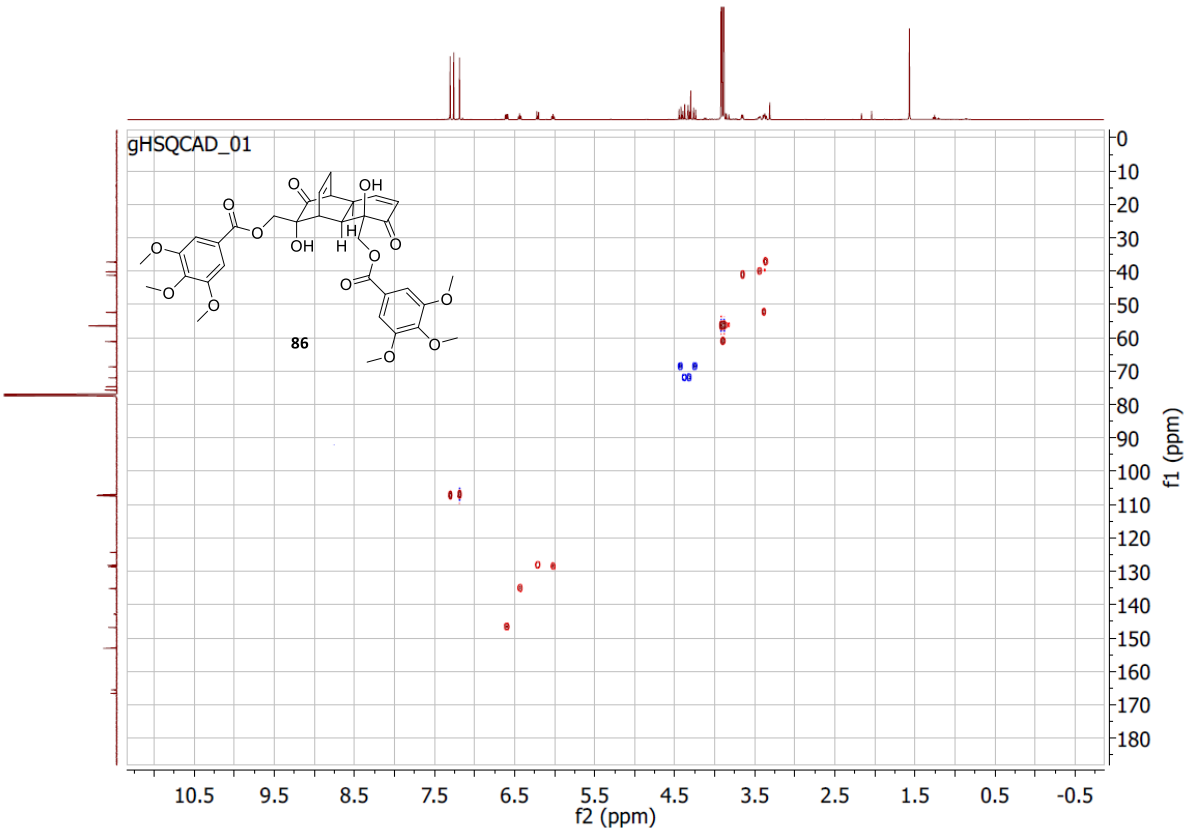


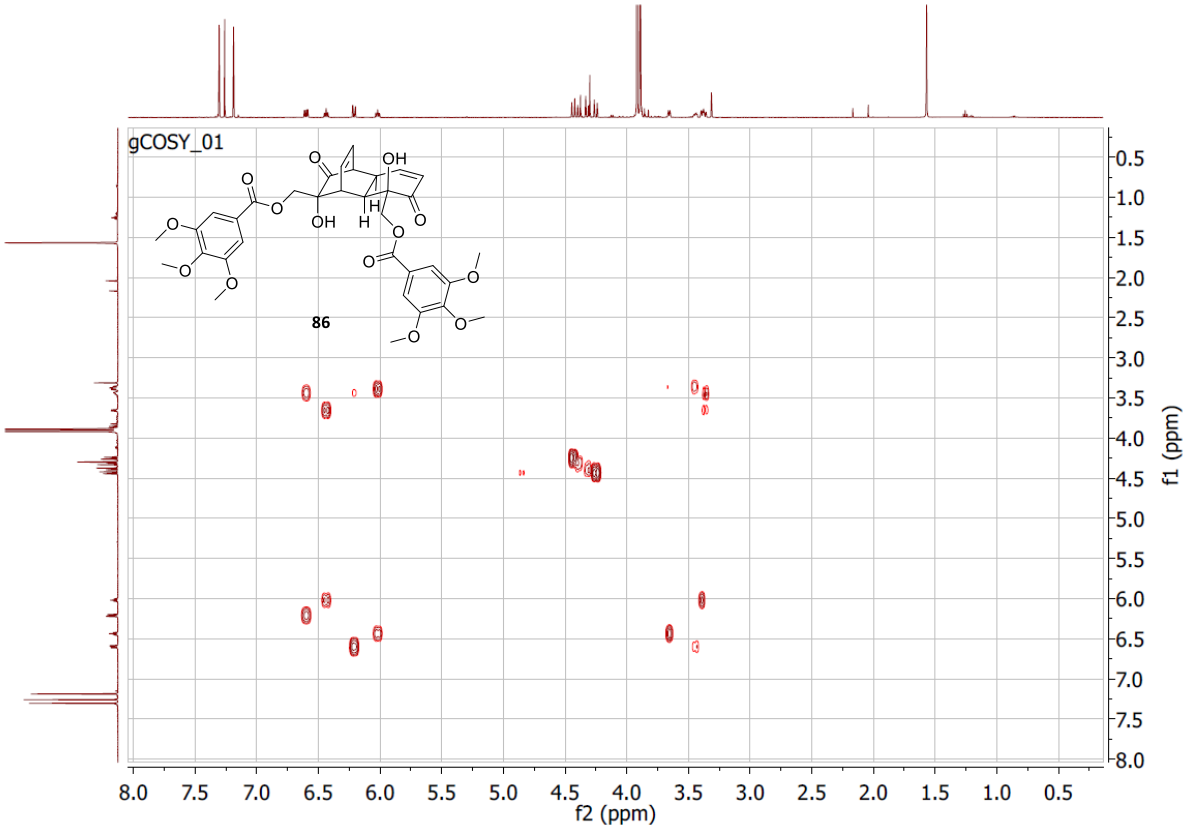
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
368.1144	1	C 20 H 18 N O 6	63.60	368.1129	-1.5	-4.1	5.1	12.5	even	ok
	2	C 17 H 10 N 11	20.35	368.1115	-2.9	-7.8	8.5	18.5	even	ok
	3	C 21 H 14 N 5 O 2	100.00	368.1142	-0.2	-0.5	19.3	17.5	even	ok
	4	C 26 H 14 N 3	2.92	368.1182	3.9	10.5	46.6	21.5	even	ok

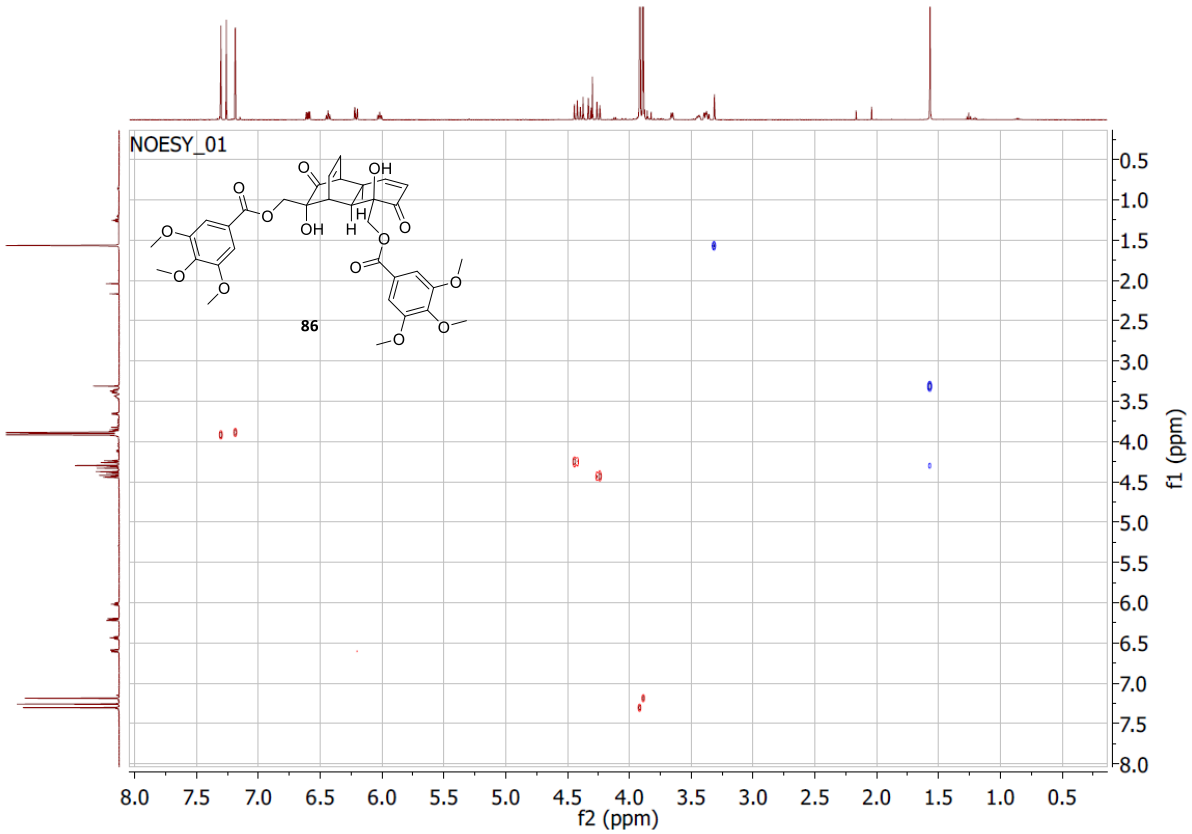

PROTON_03
J(6.65, 1.90)
E (d)
4.38
J(11.11)
Q (dd)
6.60
J(10.13, 4.26)
F (s)
3.92
B (s)
4.30
H (s)
3.89
O (dd)
6.21
J(10.10, 1.64)
S (s)
7.30
L (m)
3.38
R (s)
7.18
N (ddd)
6.02
J(7.83, 6.01, 1.37)
A (d)
4.25
J(11.86)
K (m)
3.44
M (s)
3.34
P (ddd)
6.43
J(8.05, 6.59, 1.32)
C (d)
4.32
J(11.18)
D (d)
4.43
J(11.93)
G (s)
3.91
I (s)
3.89
86
f1 (ppm)

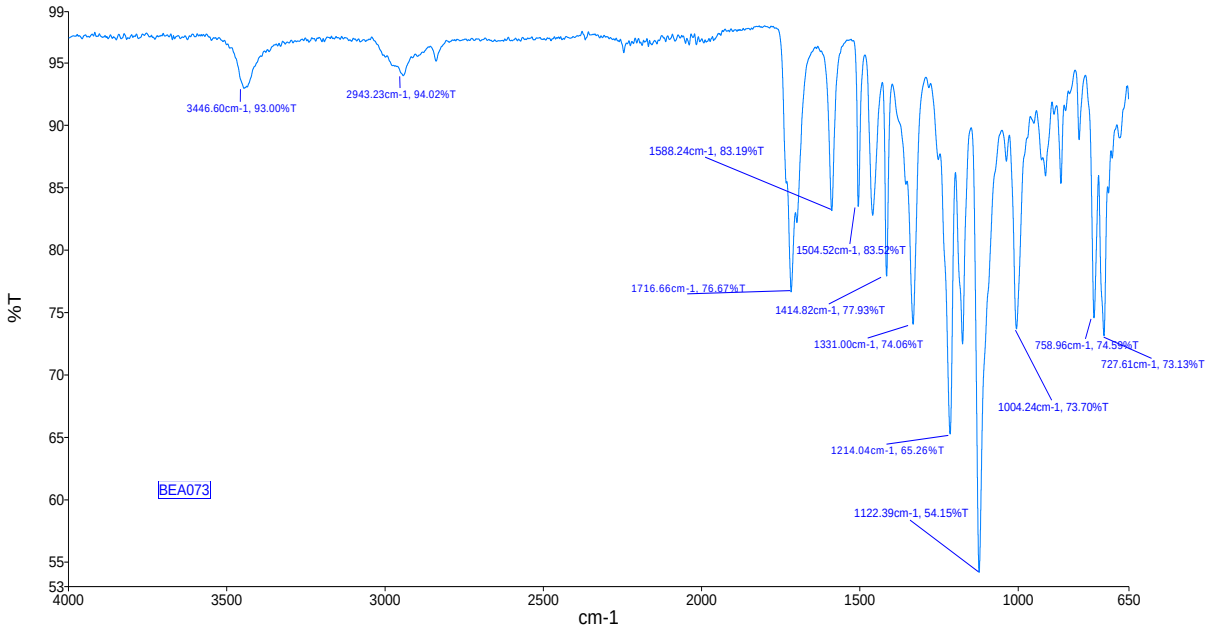

CARBON_01
166.58
165.53
153.11
146.83
142.74
135.17
128.63
128.21
124.32
107.33
107.08
75.64
74.66
72.01
68.70
61.10
56.46
56.36
52.37
41.24
40.21
37.25
86
f1 (ppm)


gHMBCAD_01
86
f2 (ppm)
f1 (ppm)


gHSQCAD_01
86
f2 (ppm)
f1 (ppm)


gCOSY_01
86
f2 (ppm)
f1 (ppm)

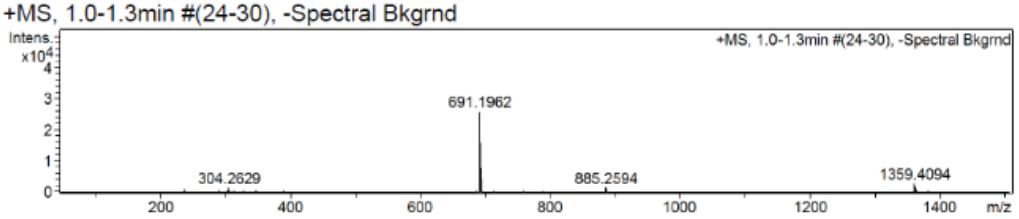

NOESY_01
86
f2 (ppm)
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_I-BEA073	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_I-BEA073_347653_26_01_52426.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to1500 loop inj.m	Acquisition Date	10/05/2016 16:30:56
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(24-30), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	236.1107	958	3.7	10	2346.9
2	304.2629	1579	6.1	109	2029.8
3	691.1962	25983	100.0	2736	3203.9
4	692.2067	7858	30.2	881	976.1
5	693.2067	1491	5.7	168	186.5
6	759.1886	750	2.9	85	180.6
7	885.2594	1471	5.7	211	627.7
8	1359.4094	2817	10.8	627	987.1
9	1360.4137	2057	7.9	433	727.8
10	1361.4134	734	2.8	171	262.2

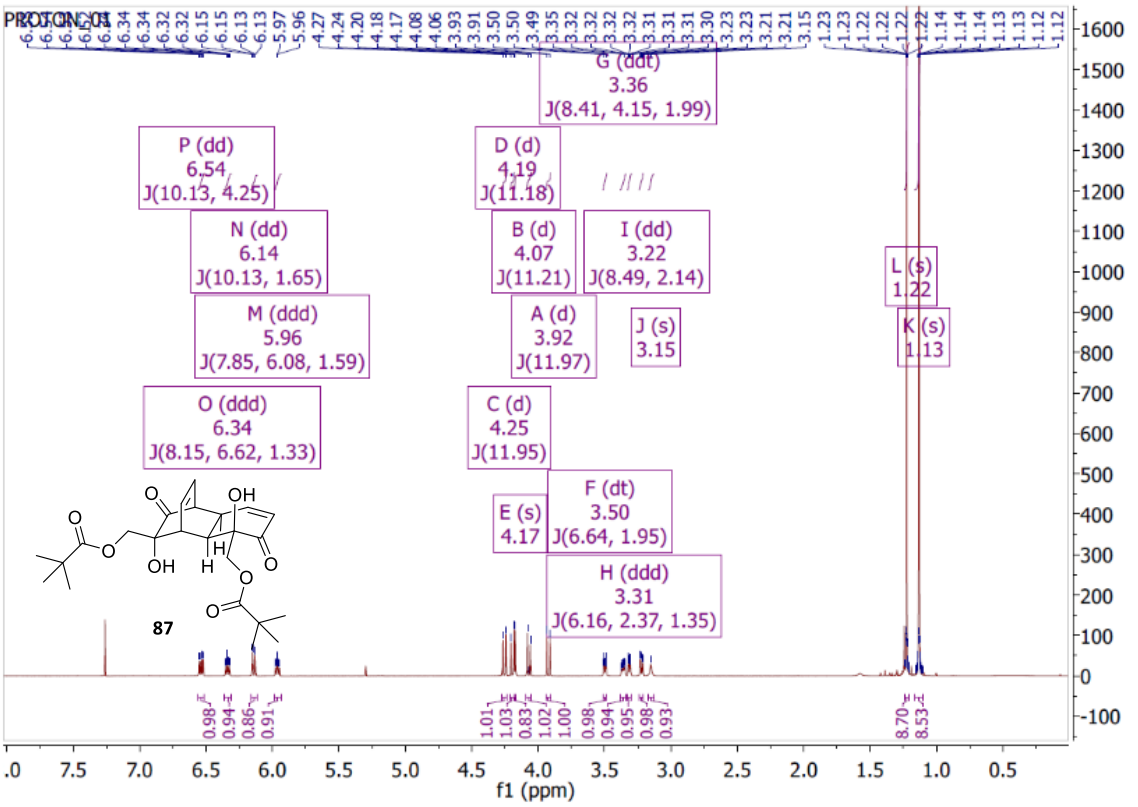
Generate Molecular Formula Parameters

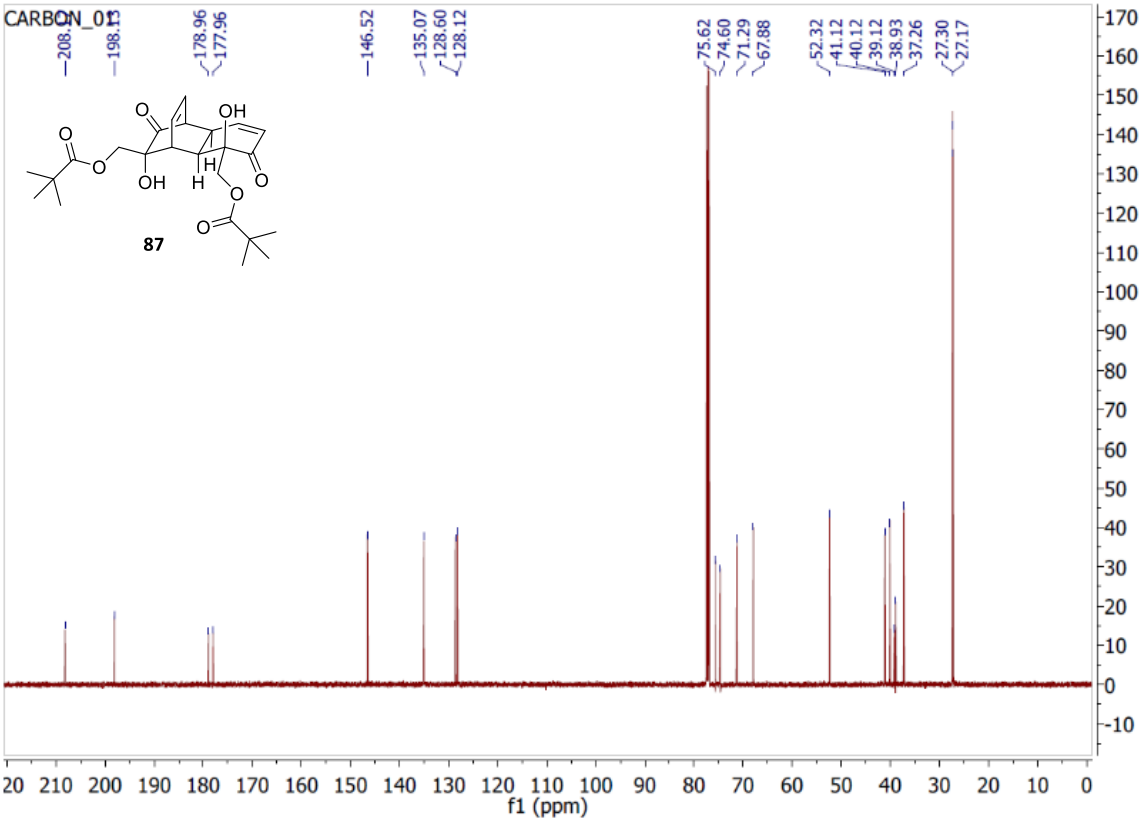
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

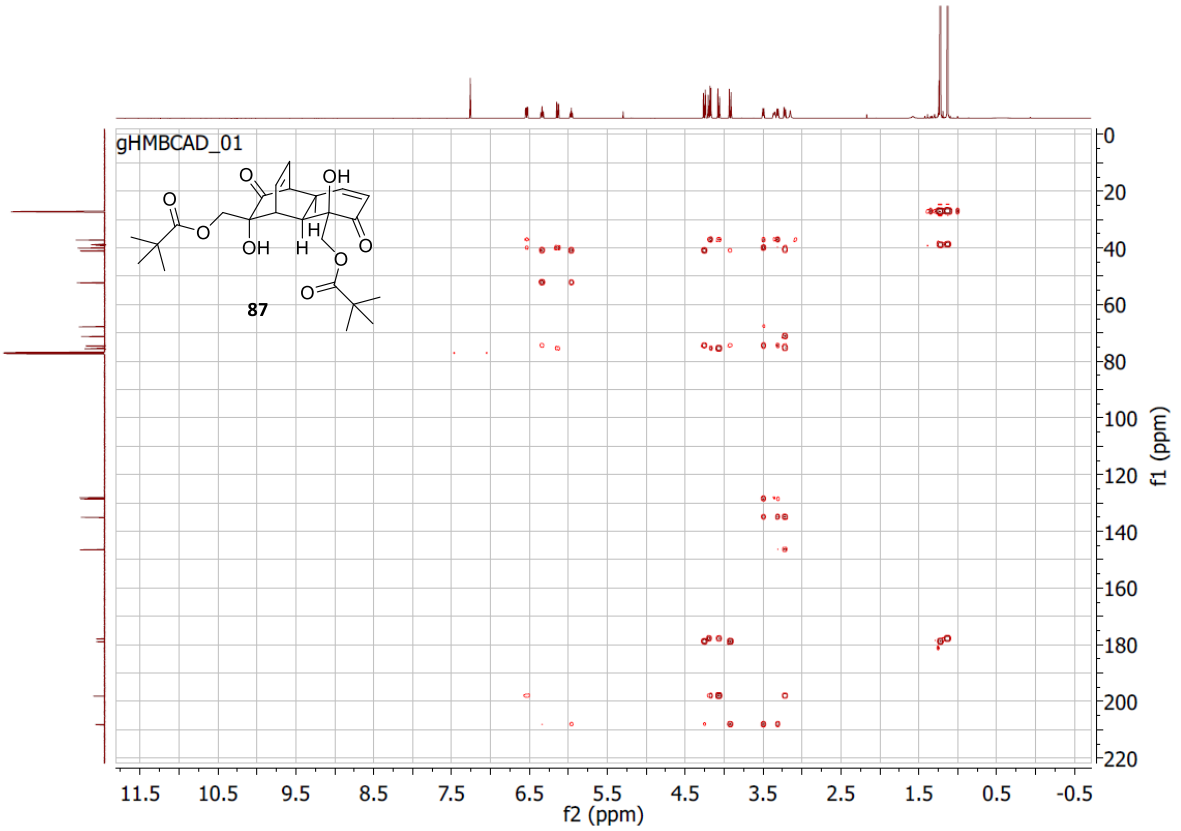
Expected Formula C34 H36 O14 **Adduct(s):** H, Na

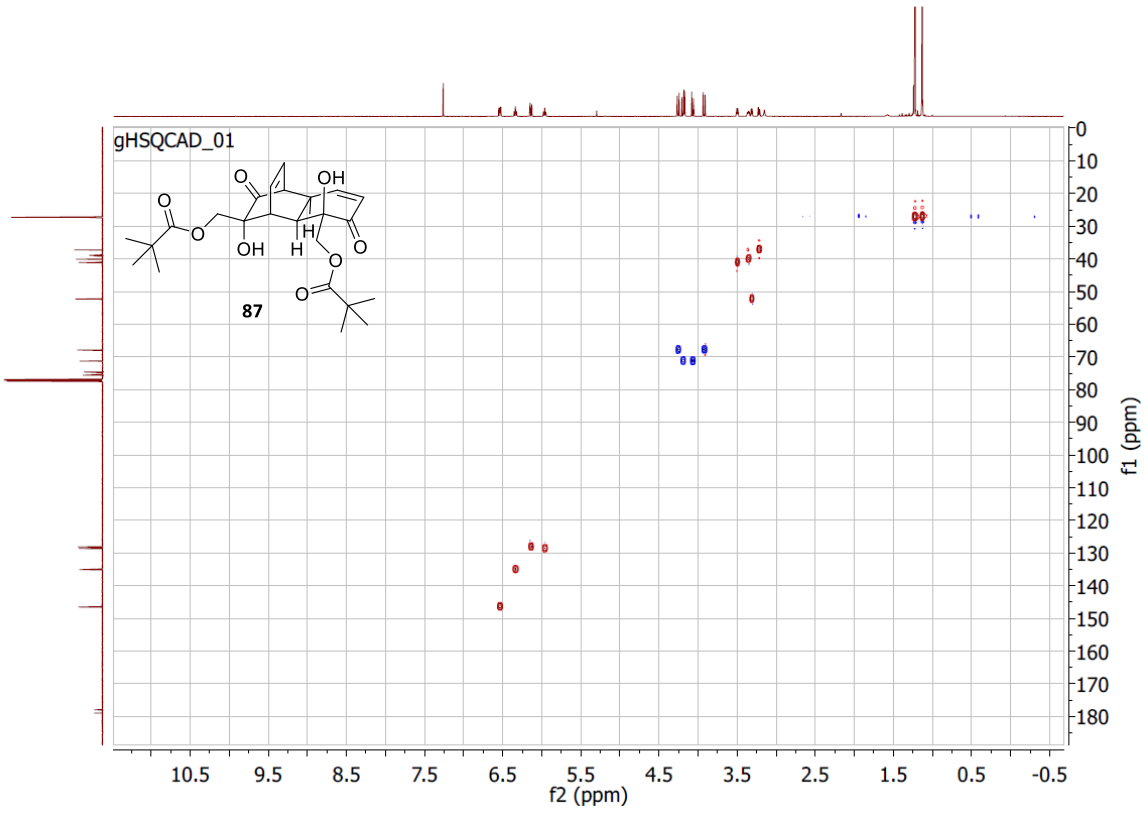
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	691.1962	691.200276	5.10	0.0429	C 34 H 36 Na 1 O 14

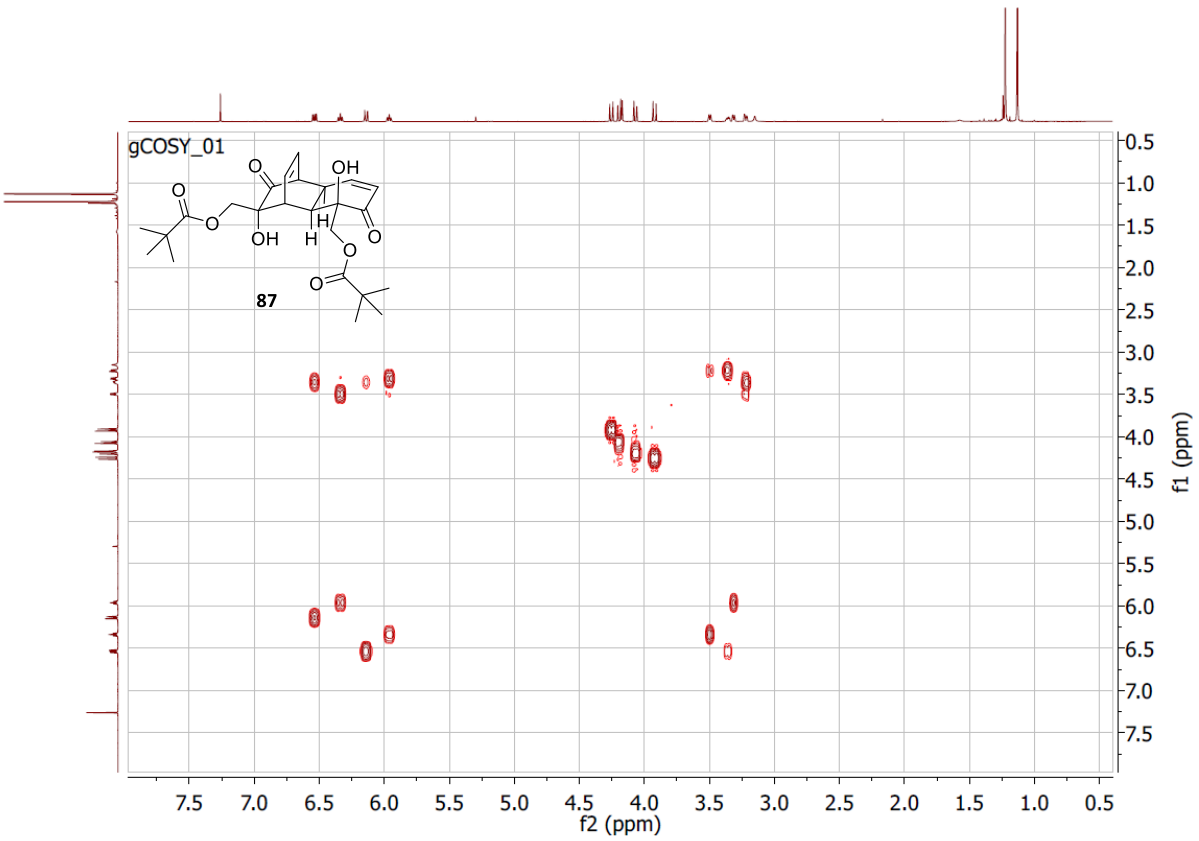
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

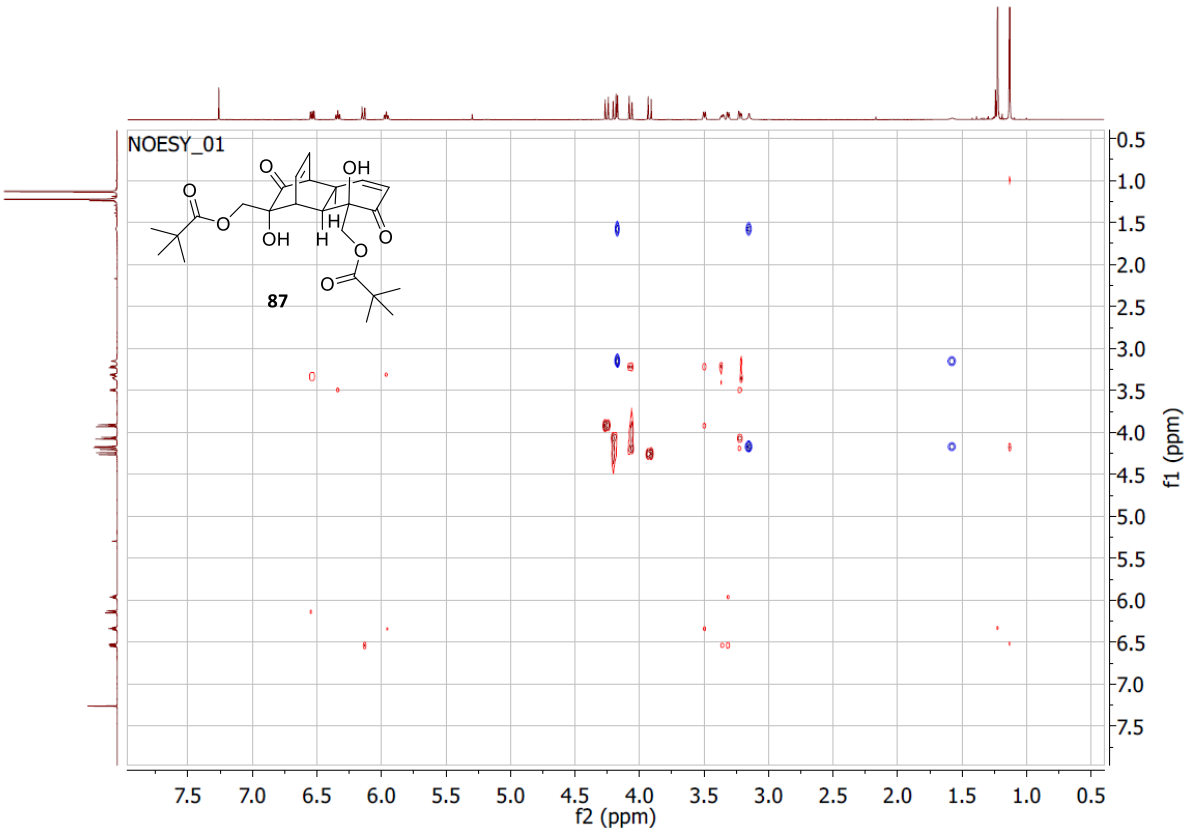

PROTON_01
G (ddt)
3.36
J(8.41, 4.15, 1.99)
P (dd)
6.54
J(10.13, 4.25)
D (d)
4.19
J(11.18)
N (dd)
6.14
J(10.13, 1.65)
B (d)
4.07
J(11.21)
I (dd)
3.22
J(8.49, 2.14)
L (s)
1.22
M (ddd)
5.96
J(7.85, 6.08, 1.59)
A (d)
3.92
J(11.97)
J (s)
3.15
K (s)
1.13
O (ddd)
6.34
J(8.15, 6.62, 1.33)
C (d)
4.25
J(11.95)
F (dt)
3.50
J(6.64, 1.95)
E (s)
4.17
H (ddd)
3.31
J(6.16, 2.37, 1.35)
87
f1 (ppm)

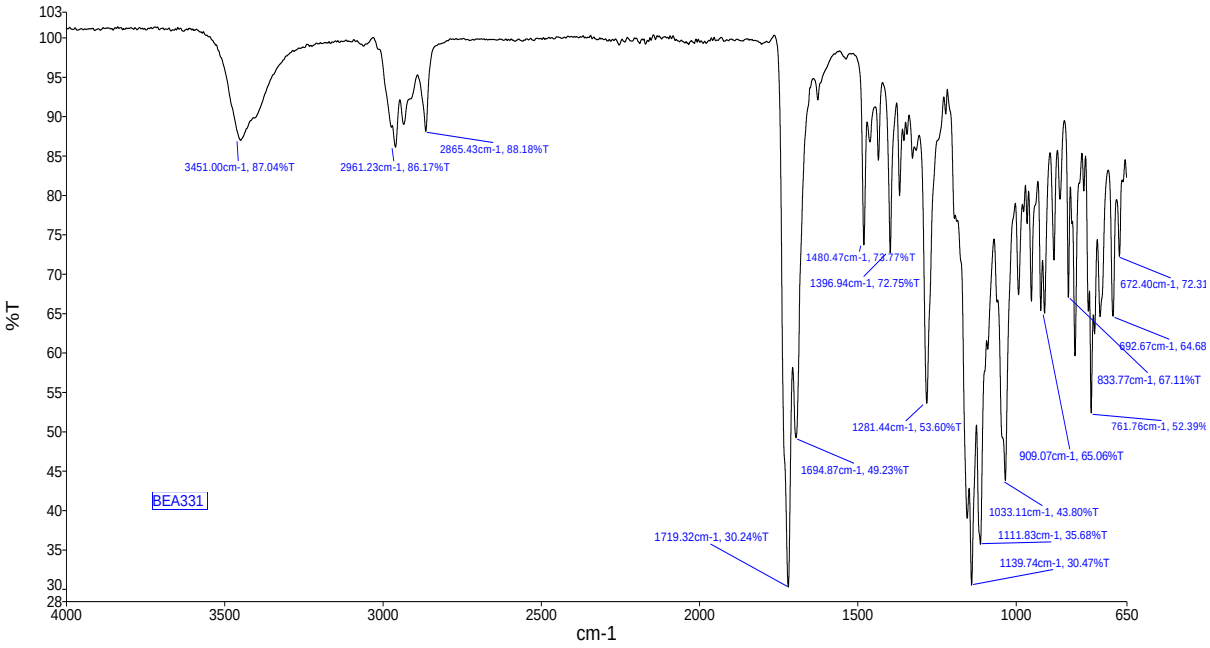

CARBON_01
87
f1 (ppm)


gHMBCAD_01
87
f2 (ppm)
f1 (ppm)


gHSQCAD_01
87
f2 (ppm)
f1 (ppm)


gCOSY_01
87
f2 (ppm)
f1 (ppm)

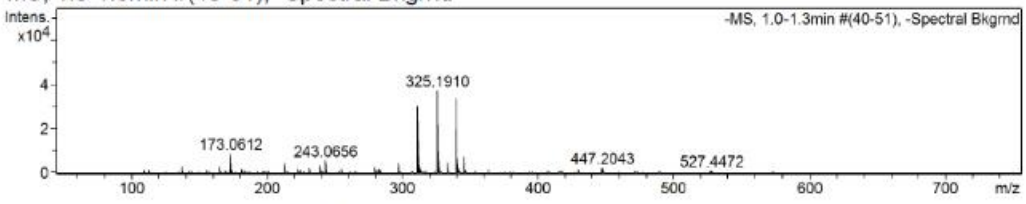

NOESY_01
87
f2 (ppm)
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_BEA331 F	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA331 F_356048_42_01_62049.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Negative 50to500 loop inj.m	Acquisition Date	27/02/2018 12:35:25
Ionisation Mode	negative electrospray (ESI)		

-MS, 1.0-1.3min #(40-51), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	173.0612	8677	23.5	315	1302.8
2	243.0656	5532	15.0	261	814.8
3	297.1576	4622	12.5	172	231.5
4	311.1761	30225	81.8	1152	1403.8
5	325.1910	36966	100.0	1534	1940.4
6	326.1937	9957	26.9	323	527.6
7	333.1345	4846	13.1	277	274.6
8	339.2061	33805	91.5	1338	2040.2
9	340.2100	7048	19.1	286	430.0
10	345.1341	7565	20.5	466	487.5

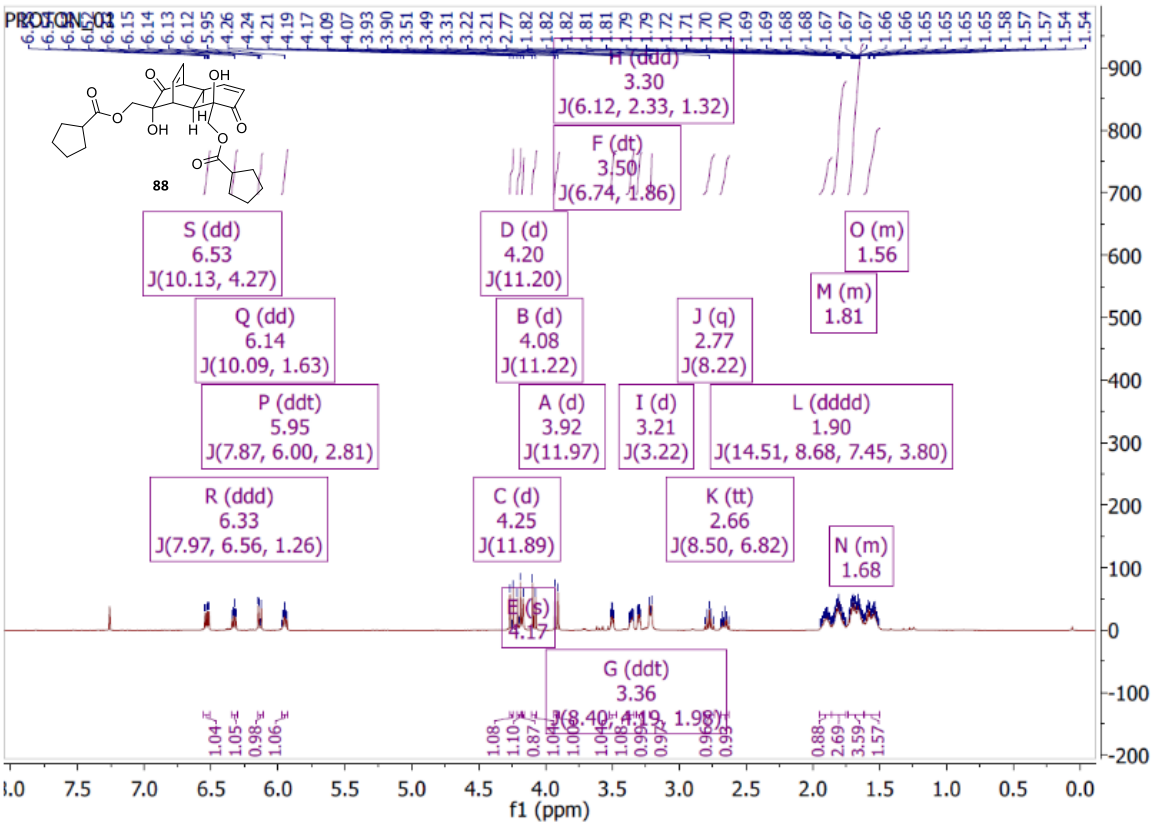
Generate Molecular Formula Parameters

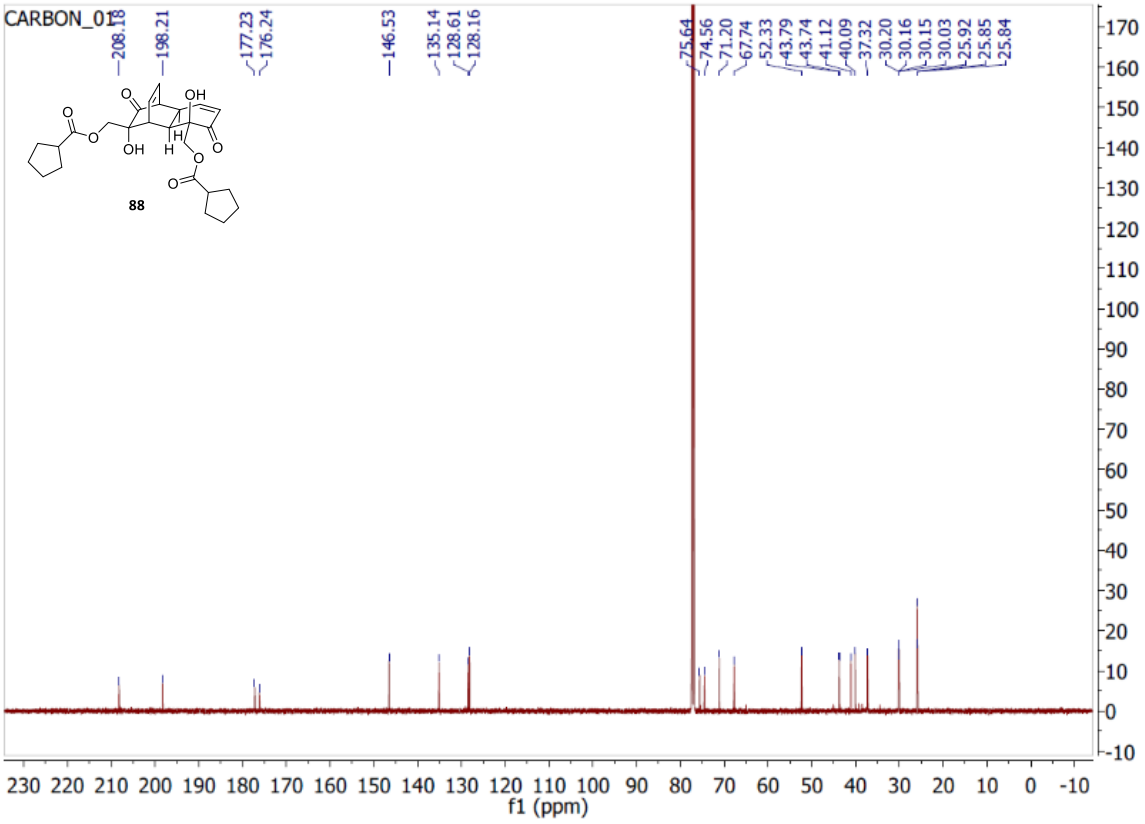
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
negative	10 ppm	0.05 m/z	0	3	both	true	0.05

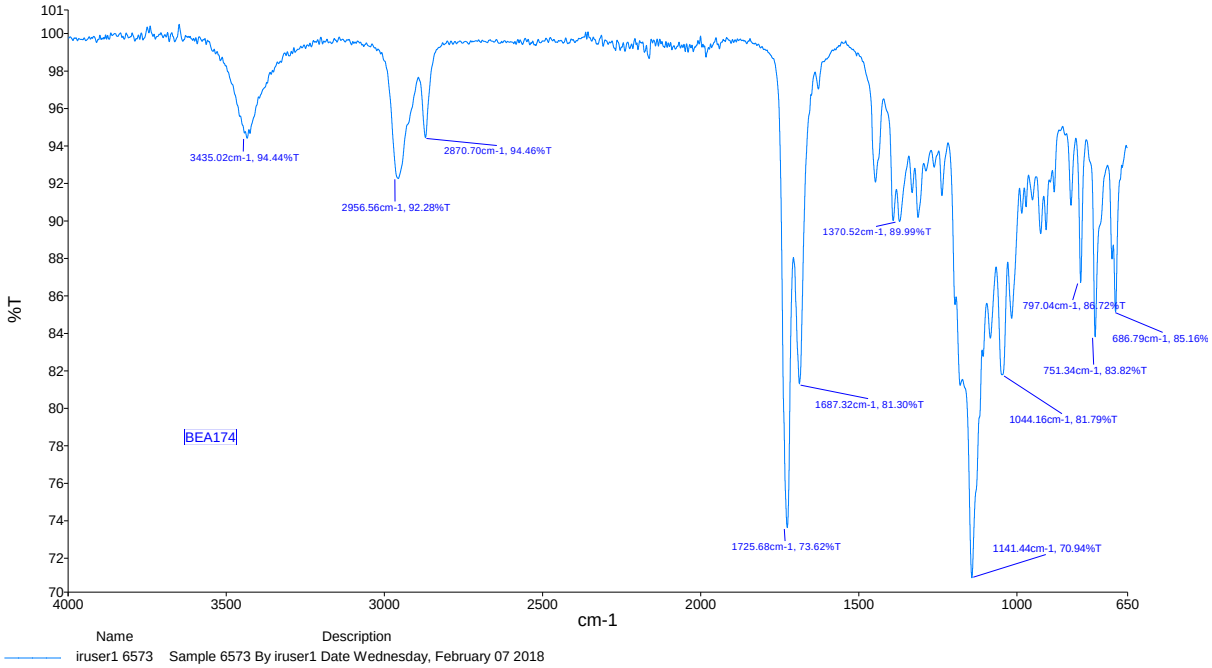
Expected Formula C24 H32 O8 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	447.2043	447.2024	4.10	0.0349	C 24 H 31 O 8
1	471.2045	471.2000	9.40	0.0251	C 24 H 32 Na 1 O 8

Note: Sigma fits < 0.05 indicates high probability of correct MF.


PROTON_01
88
H (ddd)
3.30
J(6.12, 2.33, 1.32)
F (dt)
3.50
J(6.74, 1.86)
S (dd)
6.53
J(10.13, 4.27)
D (d)
4.20
J(11.20)
O (m)
1.56
M (m)
1.81
Q (dd)
6.14
J(10.09, 1.63)
B (d)
4.08
J(11.22)
J (q)
2.77
J(8.22)
P (ddt)
5.95
J(7.87, 6.00, 2.81)
A (d)
3.92
J(11.97)
I (d)
3.21
J(3.22)
L (dddd)
1.90
J(14.51, 8.68, 7.45, 3.80)
R (ddd)
6.33
J(7.97, 6.56, 1.26)
C (d)
4.25
J(11.89)
K (tt)
2.66
J(8.50, 6.82)
N (m)
1.68
G (ddt)
3.36
f1 (ppm)

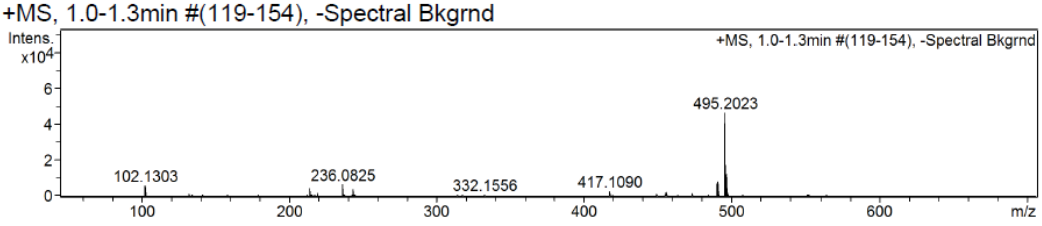

CARBON_01
88
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_BEA174 D	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA174 D_356386_73_01_62459.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	22/03/2018 15:21:58
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	102.1303	6004	13.0	122	8348.2
2	214.0936	4297	9.3	112	755.8
3	236.0825	6578	14.2	73	964.2
4	243.1375	3851	8.3	155	536.6
5	417.1090	2708	5.9	181	563.0
6	455.2114	2317	5.0	167	334.7
7	490.2460	8326	18.0	771	633.9
8	495.2023	46206	100.0	4387	3257.0
9	496.2054	12554	27.2	1185	871.8
10	497.2085	2179	4.7	190	149.1

Generate Molecular Formula Parameters

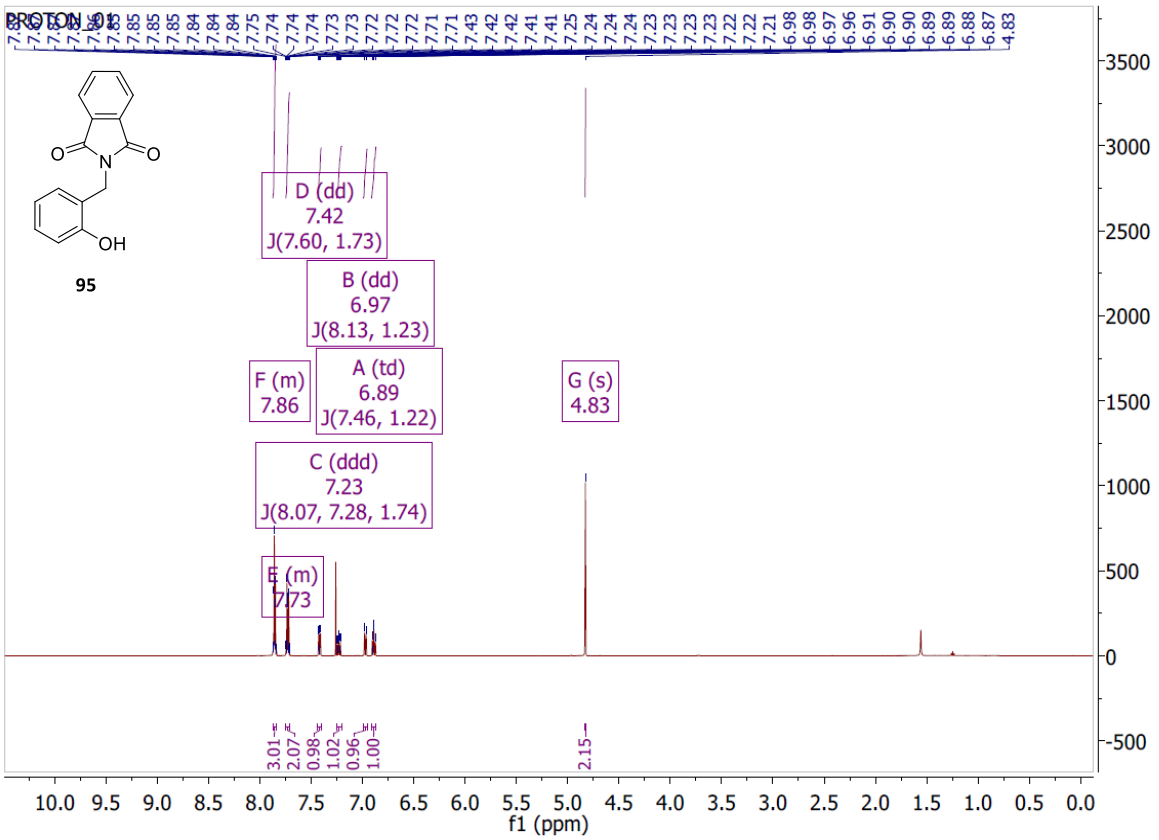
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

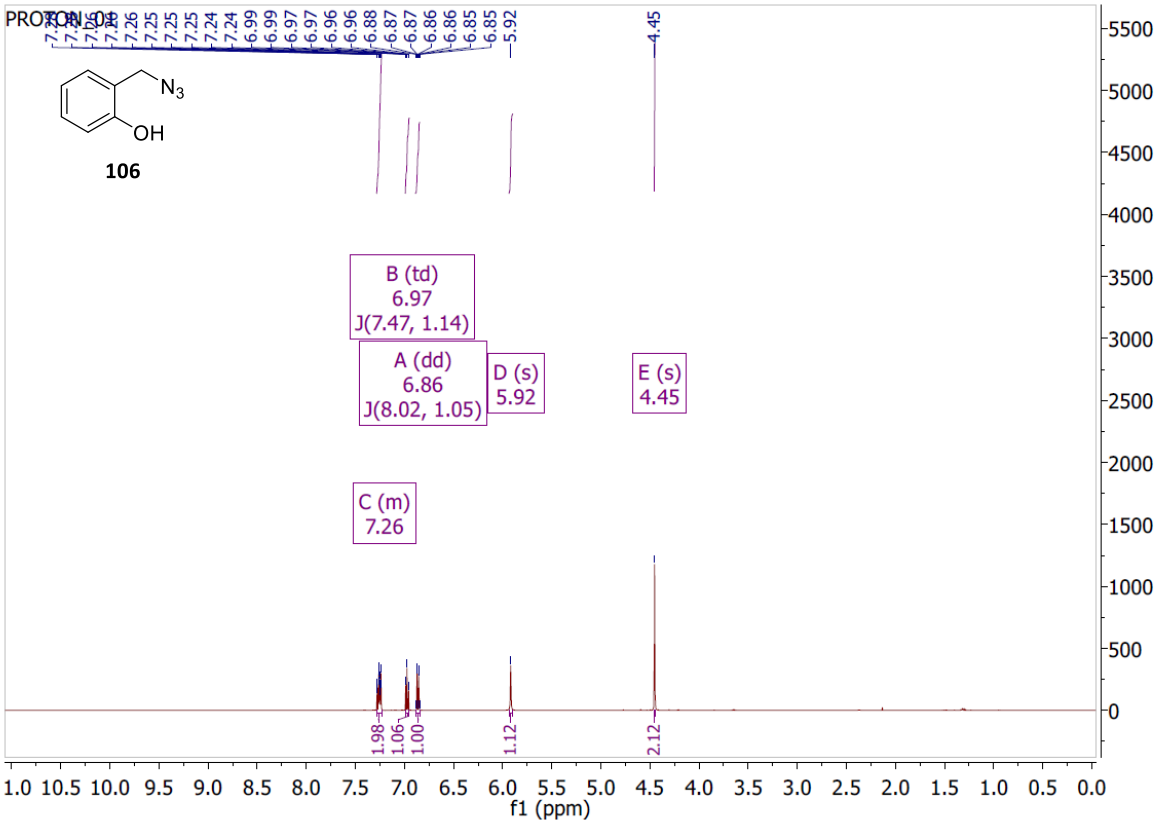
Expected Formula C26 H32 O8 **Adduct(s):** H, Na

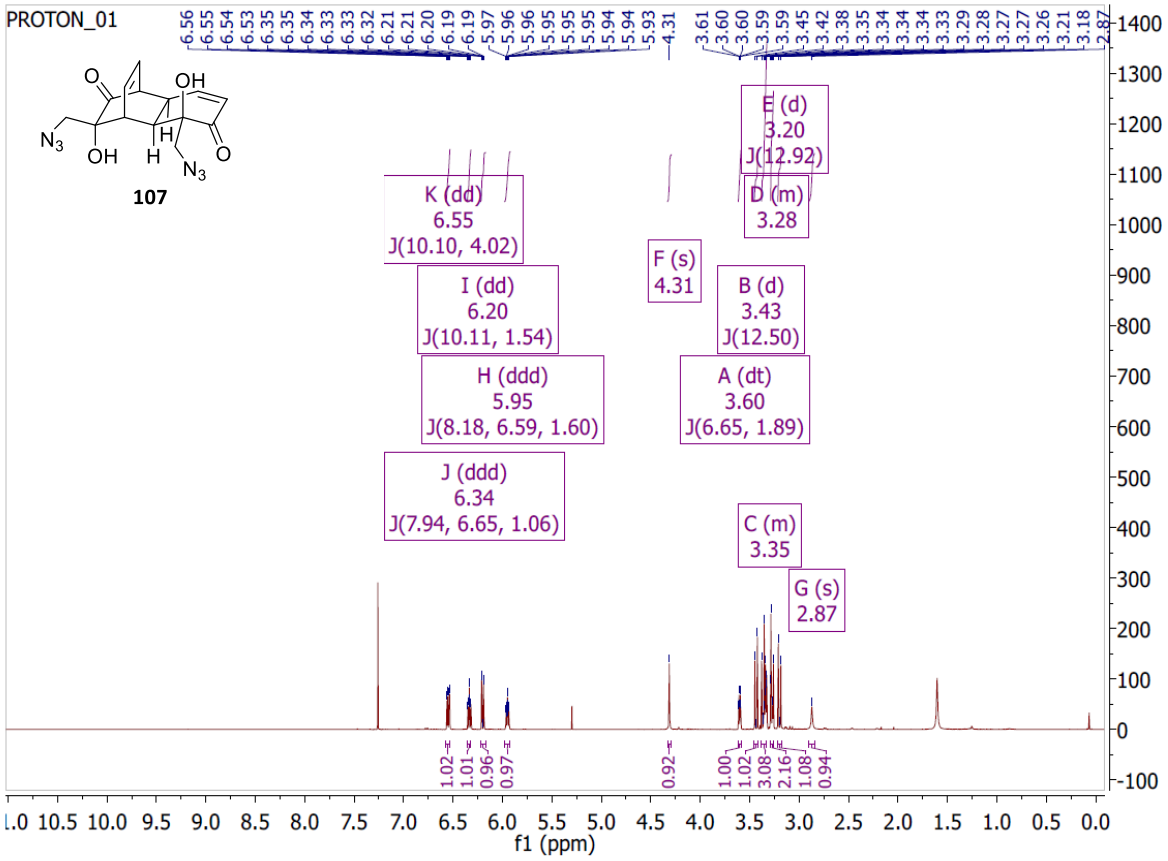
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	495.2023	495.1989	6.80	0.0078	C 26 H 32 Na 1 O 8

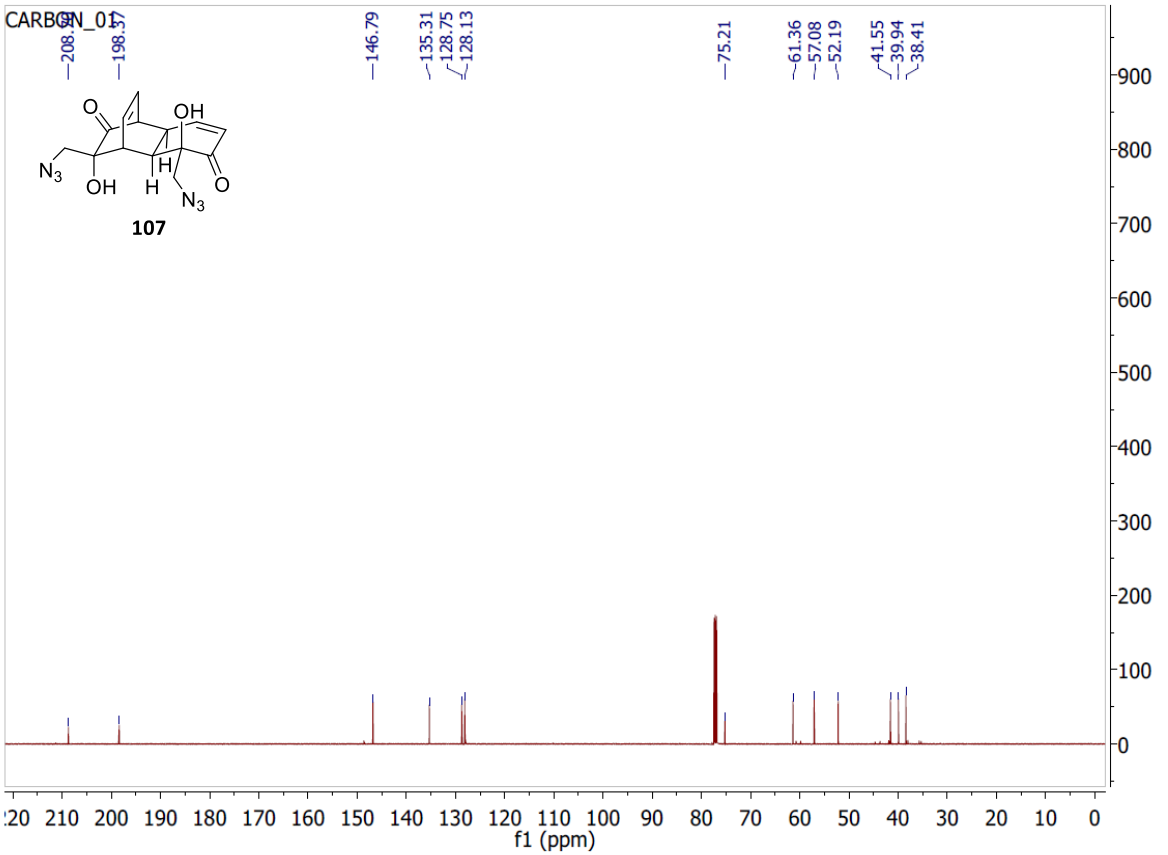
Note: Sigma fits < 0.05 indicates high probability of correct MF.

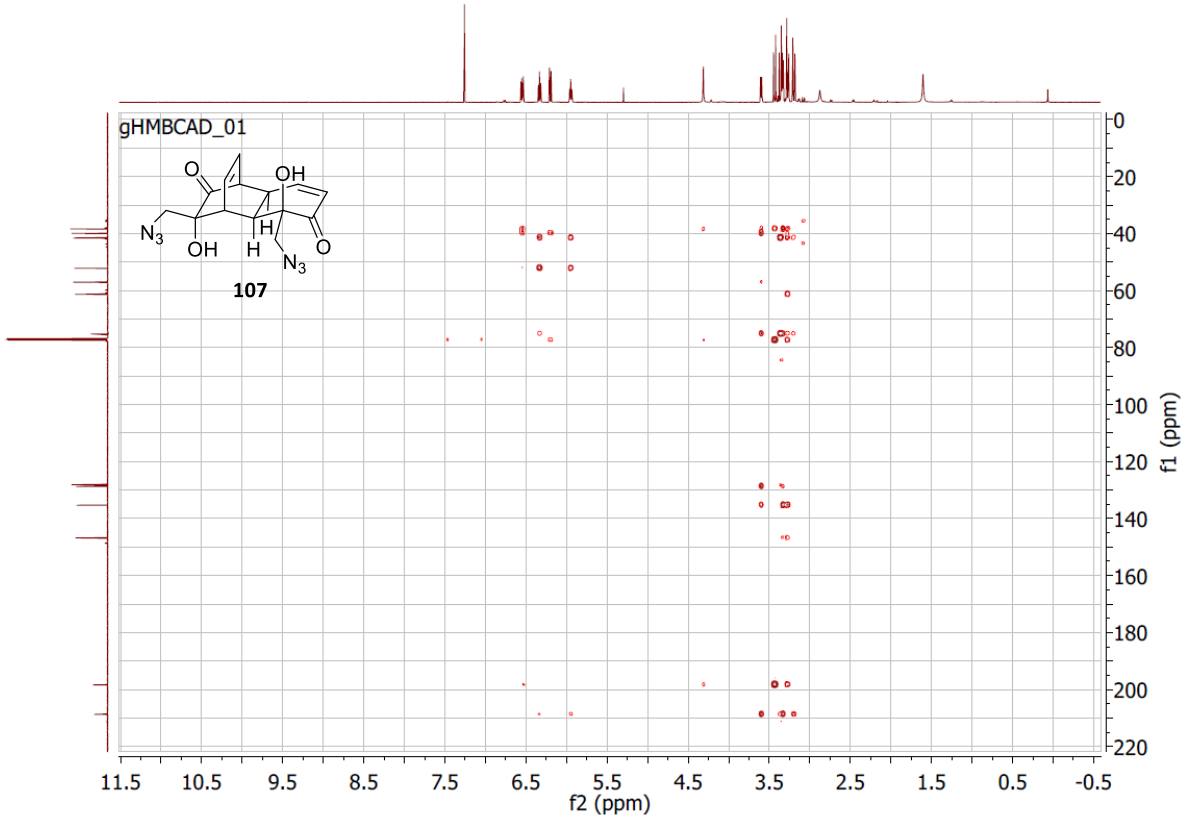
For formula confirmation the mass error / accuracy at 200 Da should be better than 25 ppm, for 500 Da better than 10 ppm and for 1000 Da better than 5 ppm

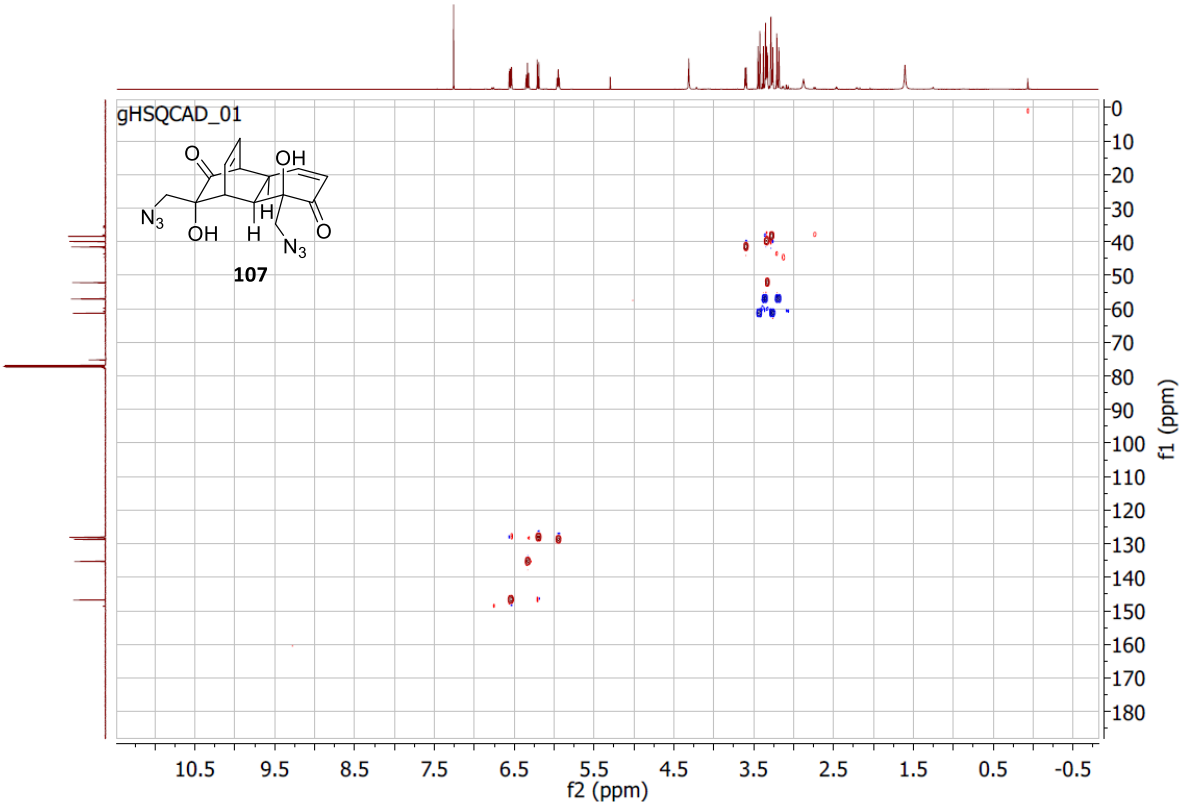

PROTON_01
95
D (dd)
7.42
J(7.60, 1.73)
B (dd)
6.97
J(8.13, 1.23)
F (m)
7.86
A (td)
6.89
J(7.46, 1.22)
G (s)
4.83
C (ddd)
7.23
J(8.07, 7.28, 1.74)
E (m)
7.73
3.01
2.07
0.98
1.02
0.96
1.00
2.15
f1 (ppm)

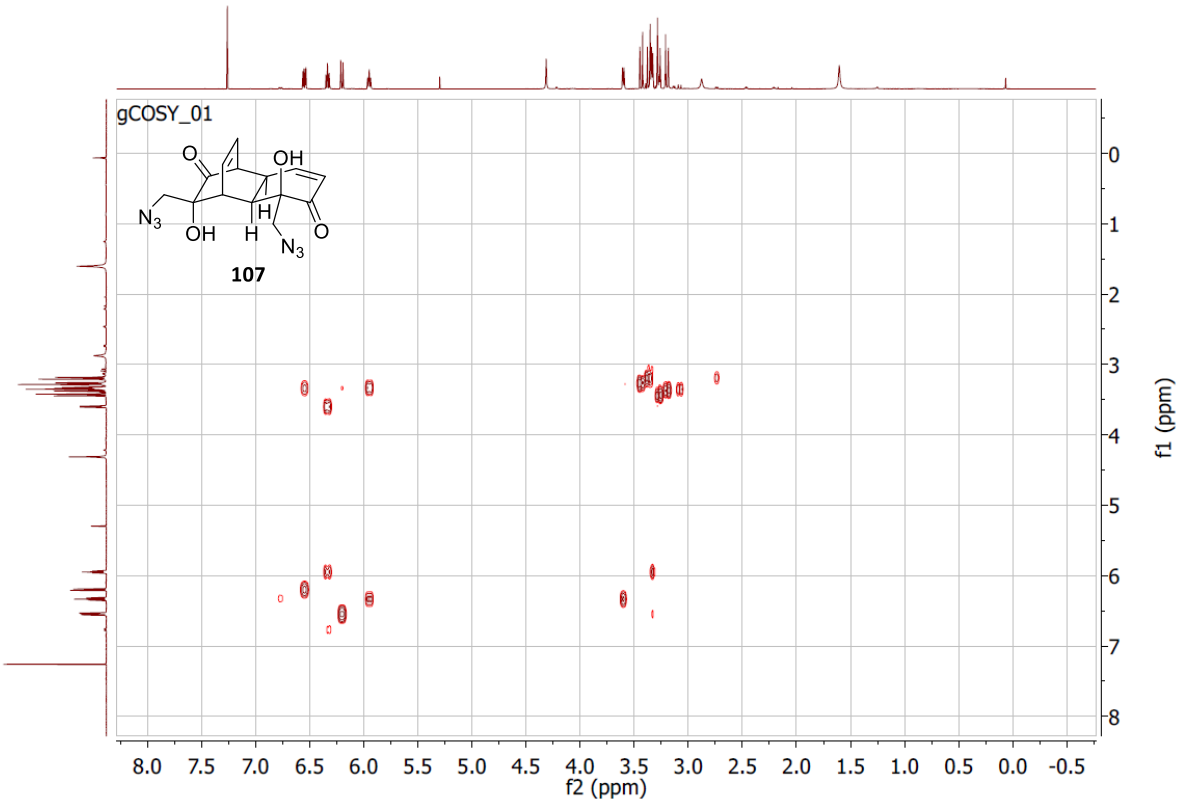

PROTON_02
106
B (td)
6.97
J(7.47, 1.14)
A (dd)
6.86
J(8.02, 1.05)
D (s)
5.92
E (s)
4.45
C (m)
7.26
1.98
1.06
1.00
1.12
2.12
f1 (ppm)

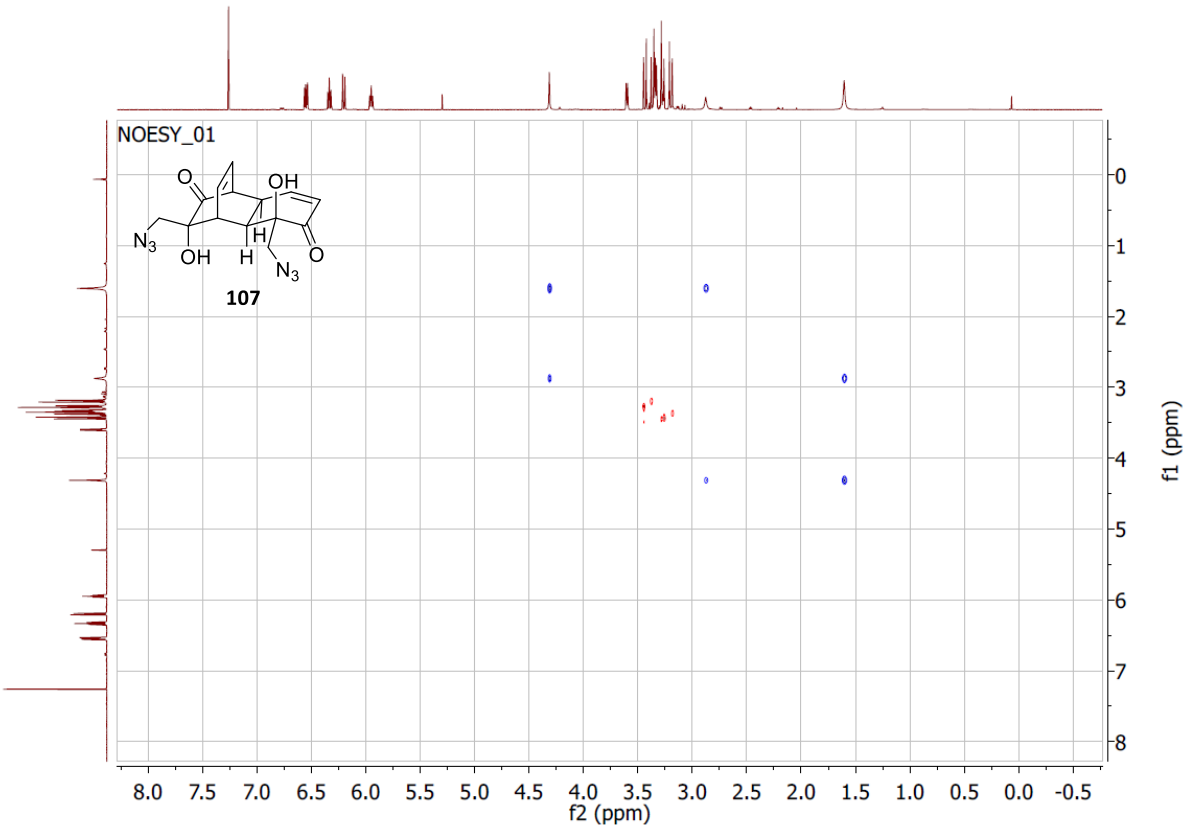

PROTON_01
107
K (dd)
6.55
J(10.10, 4.02)
I (dd)
6.20
J(10.11, 1.54)
H (ddd)
5.95
J(8.18, 6.59, 1.60)
J (ddd)
6.34
J(7.94, 6.65, 1.06)
F (s)
4.31
E (d)
3.20
J(12.92)
D (m)
3.28
B (d)
3.43
J(12.50)
A (dt)
3.60
J(6.65, 1.89)
C (m)
3.35
G (s)
2.87
f1 (ppm)

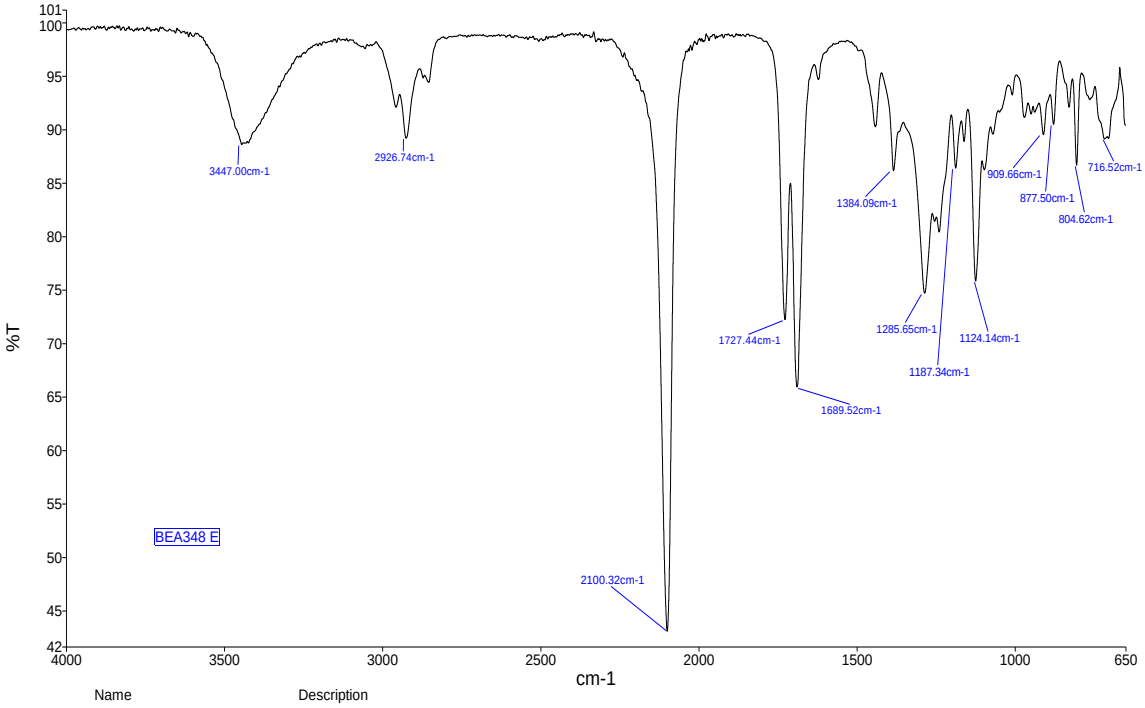

CARBON_01
107
f1 (ppm)


gHMBCAD_01
O
OH
N3
OH
H
H
N3
O
107
f2 (ppm)
f1 (ppm)


gHSQCAD_01
O
OH
N3
OH
H
H
N3
O
107
f2 (ppm)
f1 (ppm)


gCOSY_01
O
OH
N3
OH
H
H
N3
O
107
f1 (ppm)
f2 (ppm)

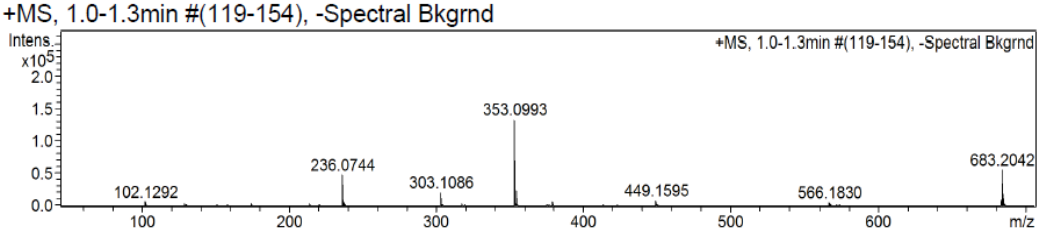

NOESY_01
O
OH
N3
OH
H
H
N3
O
107
f1 (ppm)
f2 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_BEA263D	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA263D_353278_8_01_58883.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	12/09/2017 18:03:15
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	102.1292	6285	4.7	139	2896.6
2	236.0744	47576	35.7	1578	3023.7
3	237.0805	5476	4.1	183	341.0
4	303.1086	20746	15.6	1112	1453.3
5	353.0993	133337	100.0	8481	5291.2
6	354.1014	23455	17.6	1390	916.3
7	379.1155	5986	4.5	327	186.5
8	449.1595	8355	6.3	539	695.4
9	683.2042	55598	41.7	7196	3694.4
10	684.2082	19053	14.3	2462	1265.9

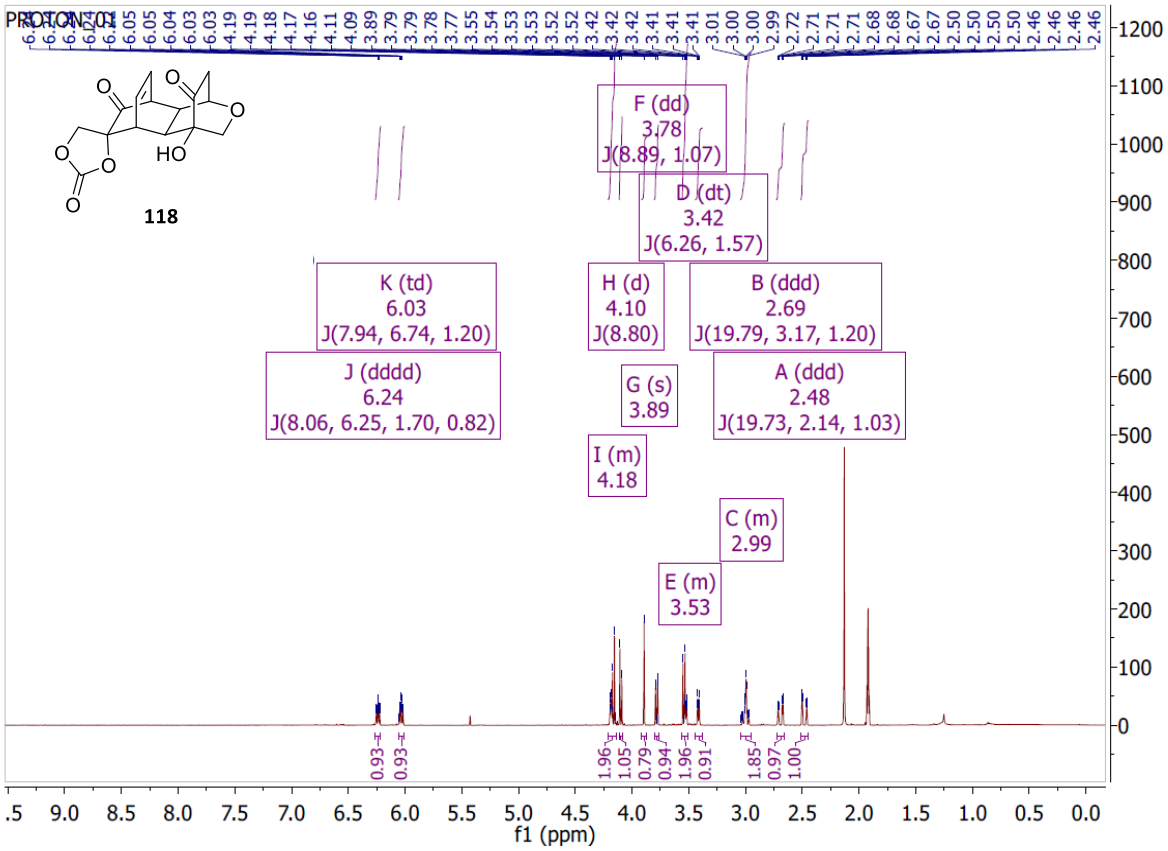
Generate Molecular Formula Parameters

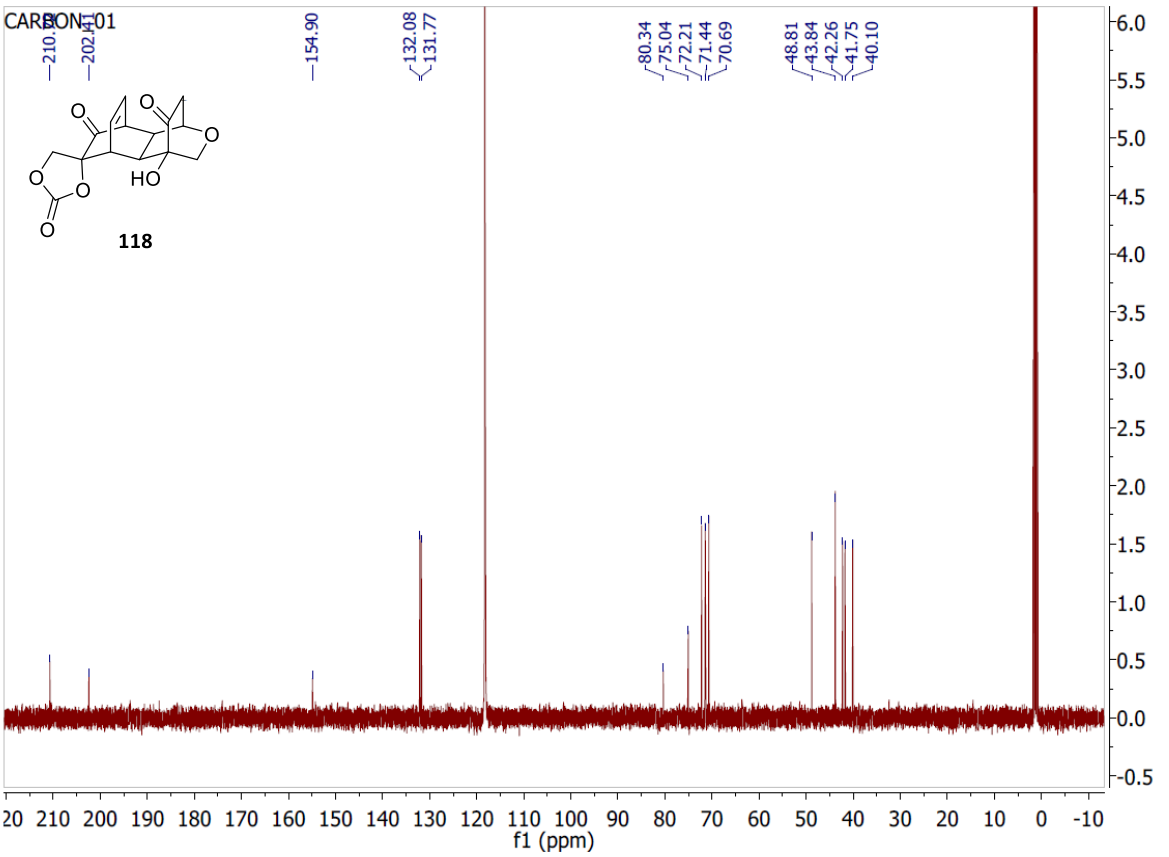
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

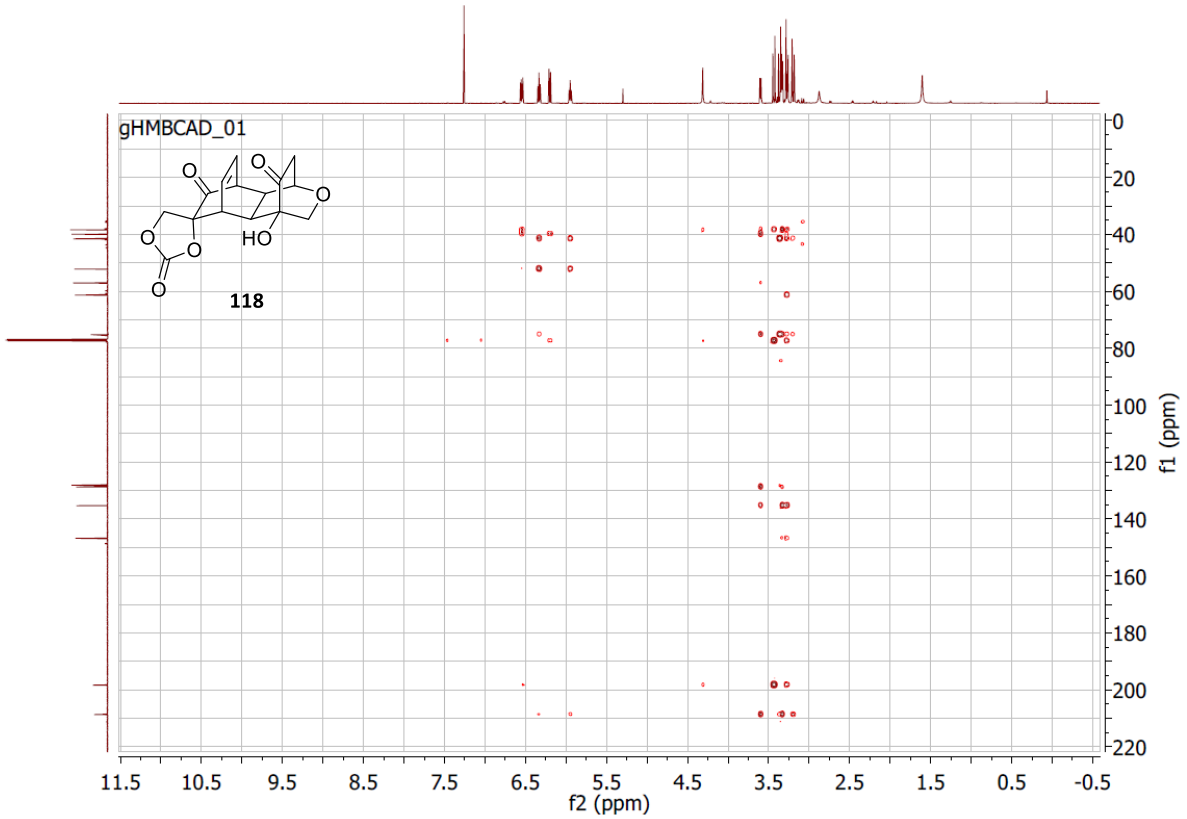
Expected Formula C14 H14 N6 O4 **Adduct(s):** H, Na

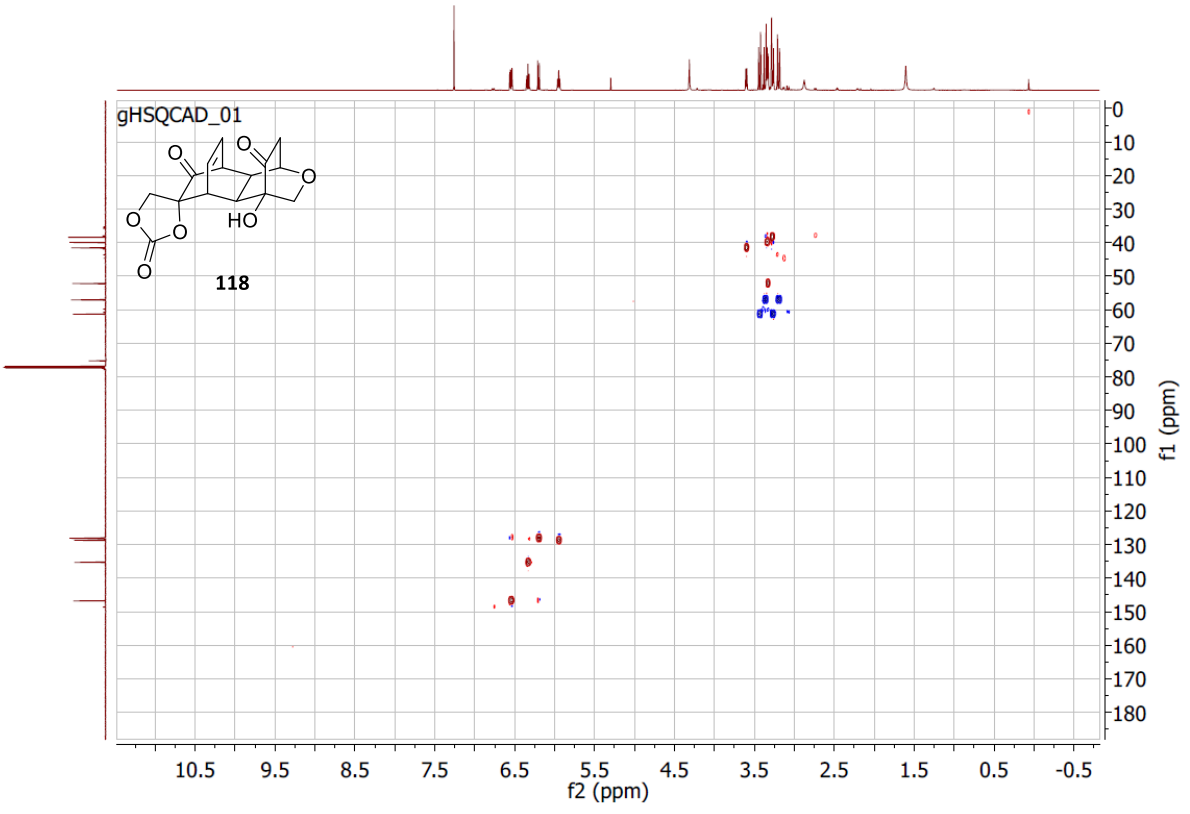
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	353.0993	353.0969	6.90	0.0043	C 14 H 14 N 6 Na 1 O 4

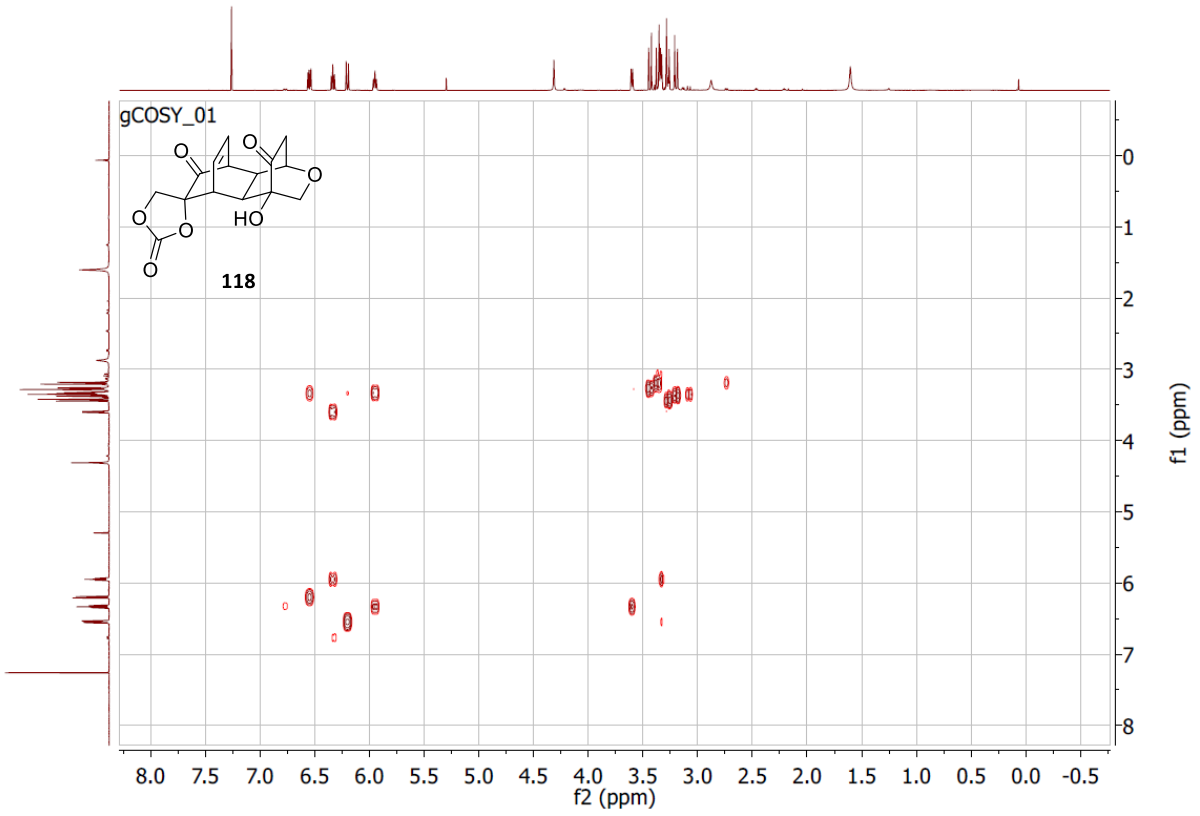
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

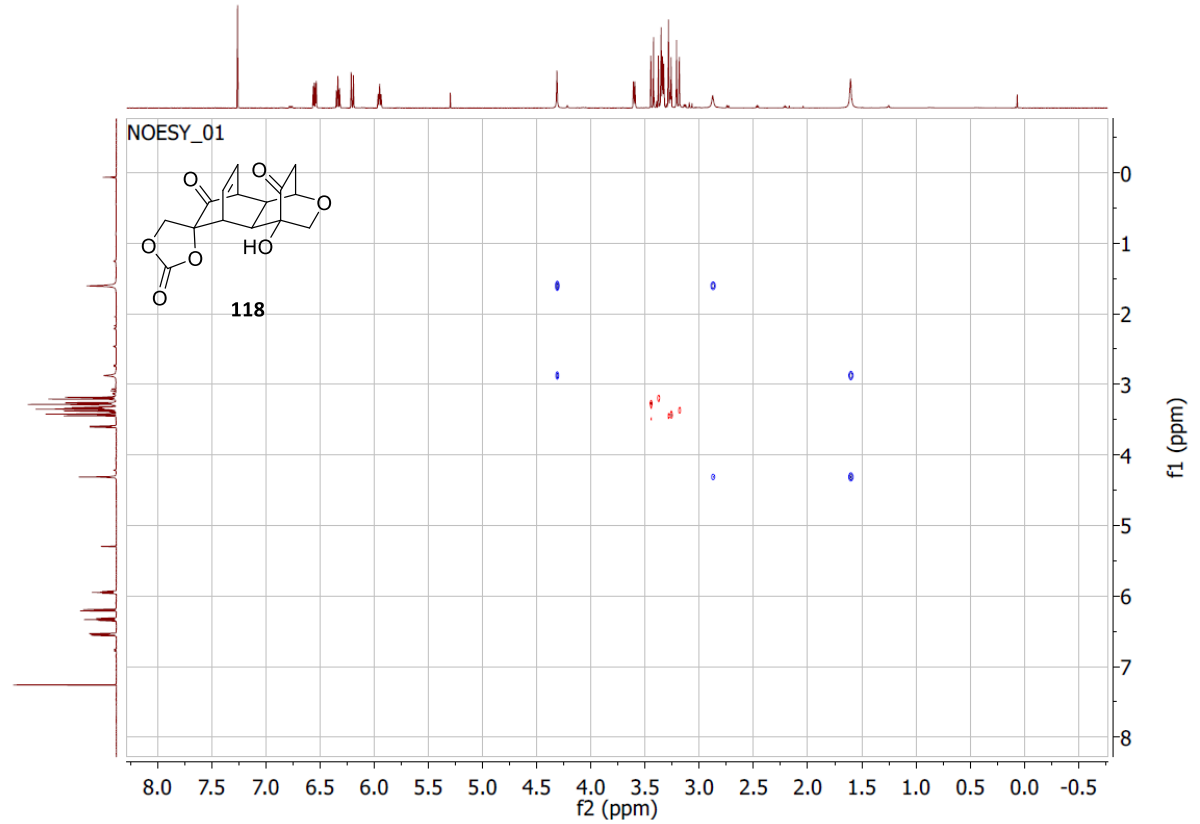

PROTON_01
HO
118
F (dd)
3.78
J(8.89, 1.07)
D (dt)
3.42
J(6.26, 1.57)
K (td)
6.03
J(7.94, 6.74, 1.20)
H (d)
4.10
J(8.80)
B (ddd)
2.69
J(19.79, 3.17, 1.20)
J (dddd)
6.24
J(8.06, 6.25, 1.70, 0.82)
G (s)
3.89
A (ddd)
2.48
J(19.73, 2.14, 1.03)
I (m)
4.18
C (m)
2.99
E (m)
3.53
f1 (ppm)

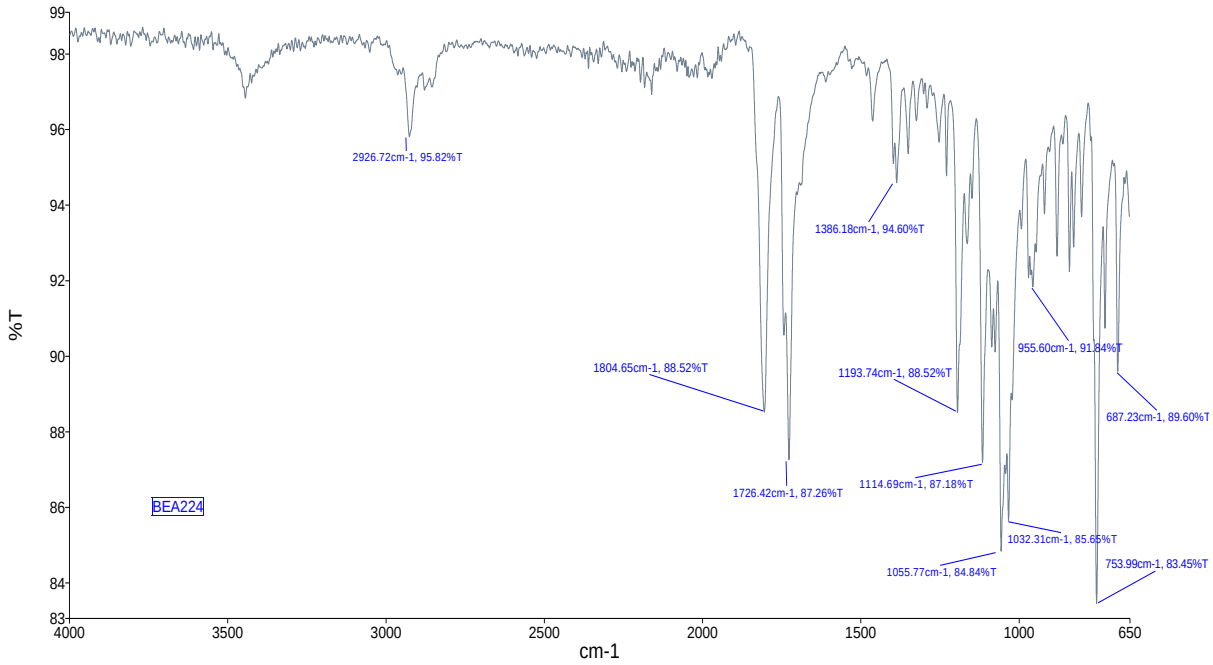

CARBON_01
HO
118
f1 (ppm)


gHMBCAD_01
HO
118
f2 (ppm)
f1 (ppm)


gHSQCAD_01
HO
118
f2 (ppm)
f1 (ppm)


gCOSY_01
HO
118
f2 (ppm)
f1 (ppm)


NOESY_01
HO
118
f2 (ppm)
f1 (ppm)



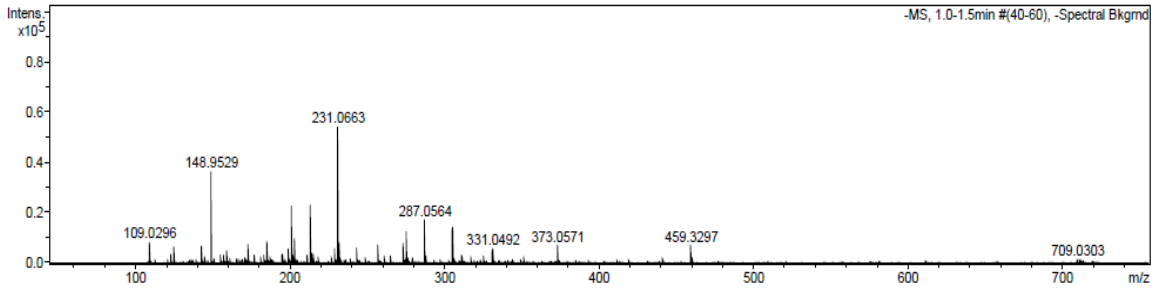
Mass Spectrum SmartFormula Report

Analysis Info

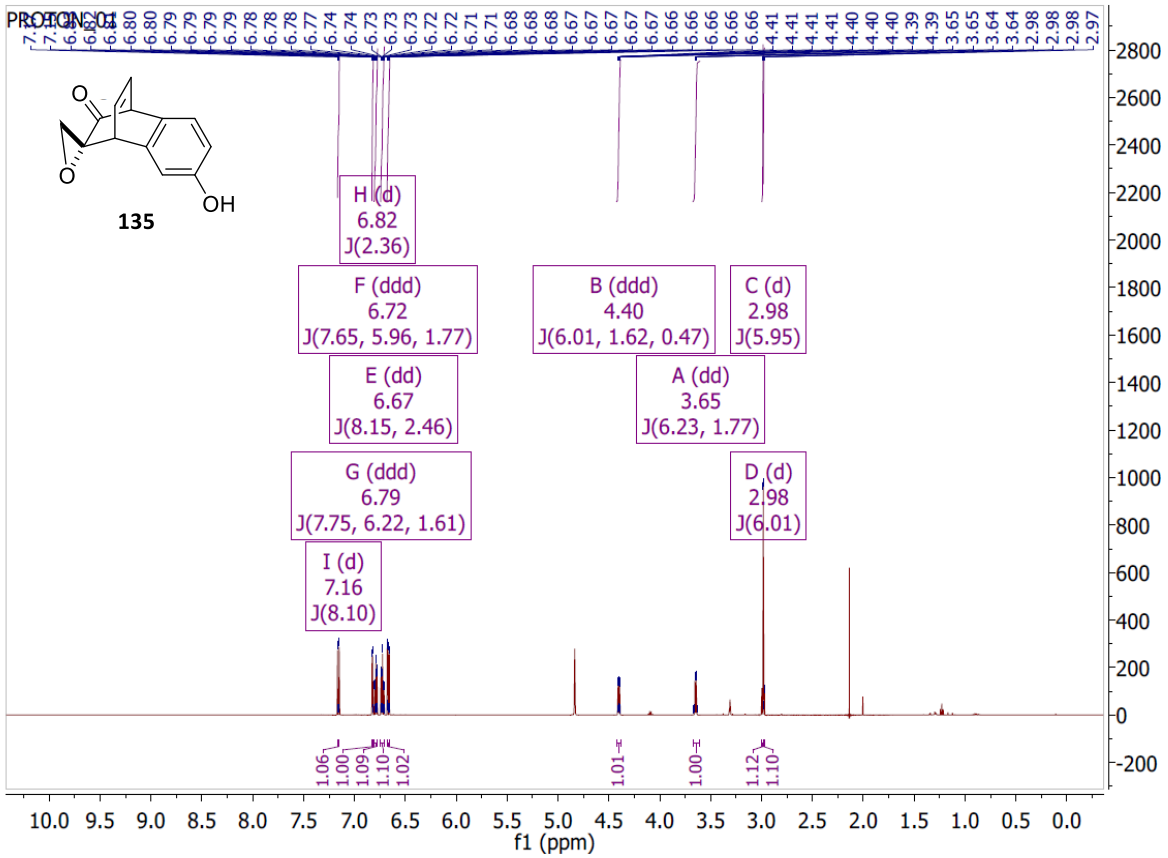
Analysis Name	Z:\ba_sel_BEA224_358358_39_01_64730.d	Acquisition Date	8/14/2018 10:47:18 AM
Method	Confirm Formula Negative 50to500 loop inj.m	Operator	admin
Sample Name	ba_sel_BEA224_358358	Instrument / Ser#	micrOTOF 161
Comment			

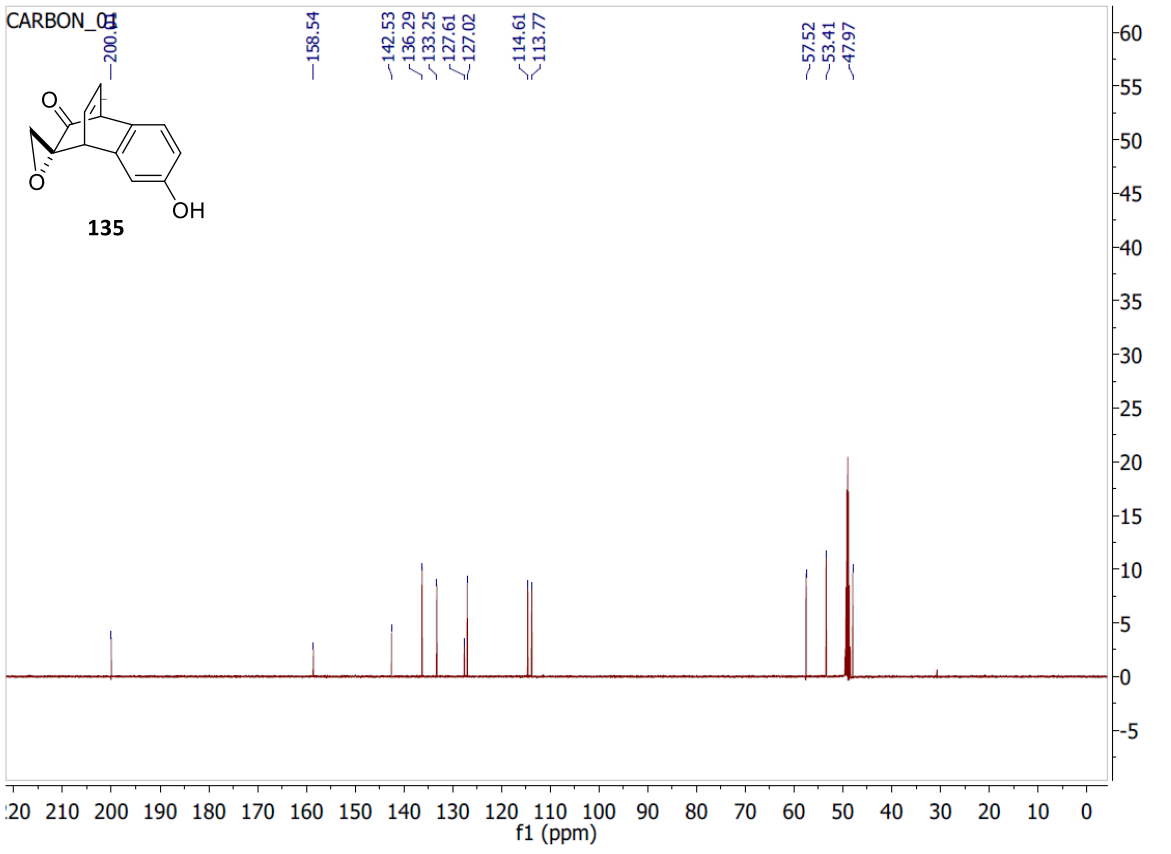
Acquisition Parameter

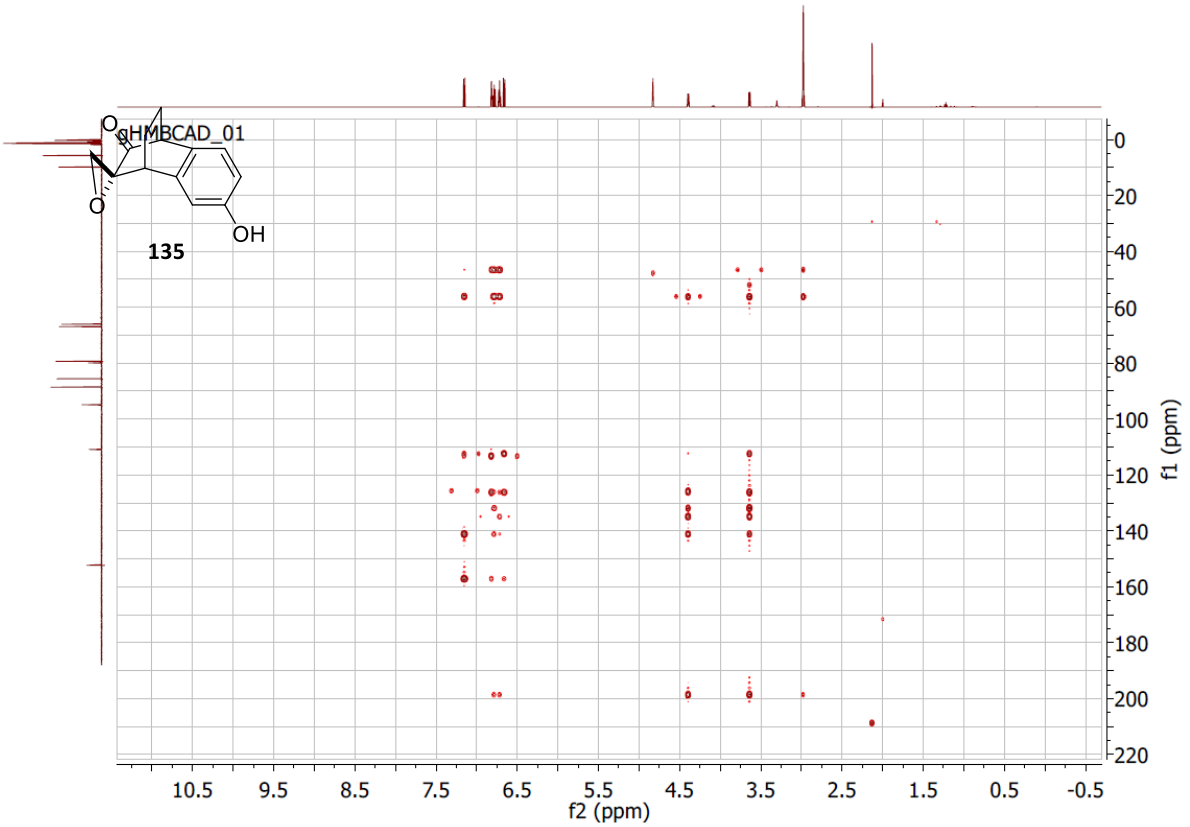
Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.2 Bar
Focus	Not active			Set Dry Heater	220 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.2 l/min
Scan End	750 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

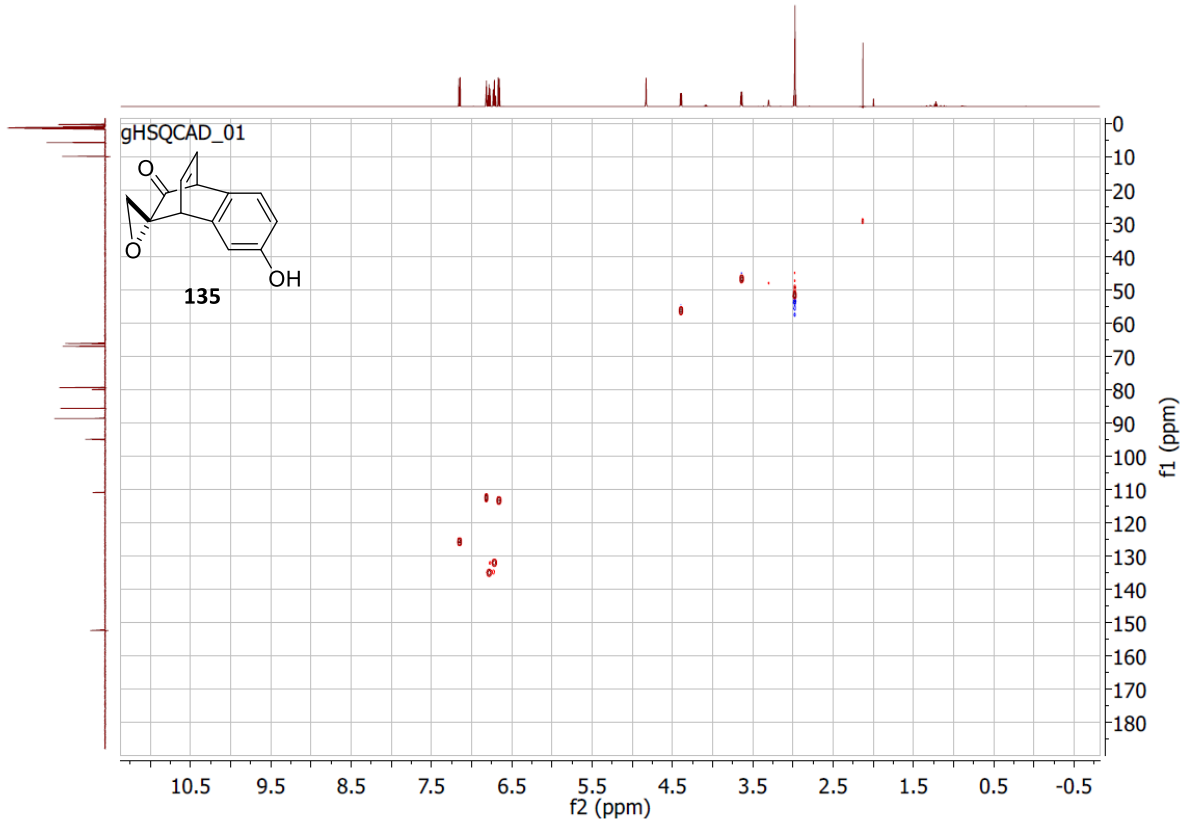


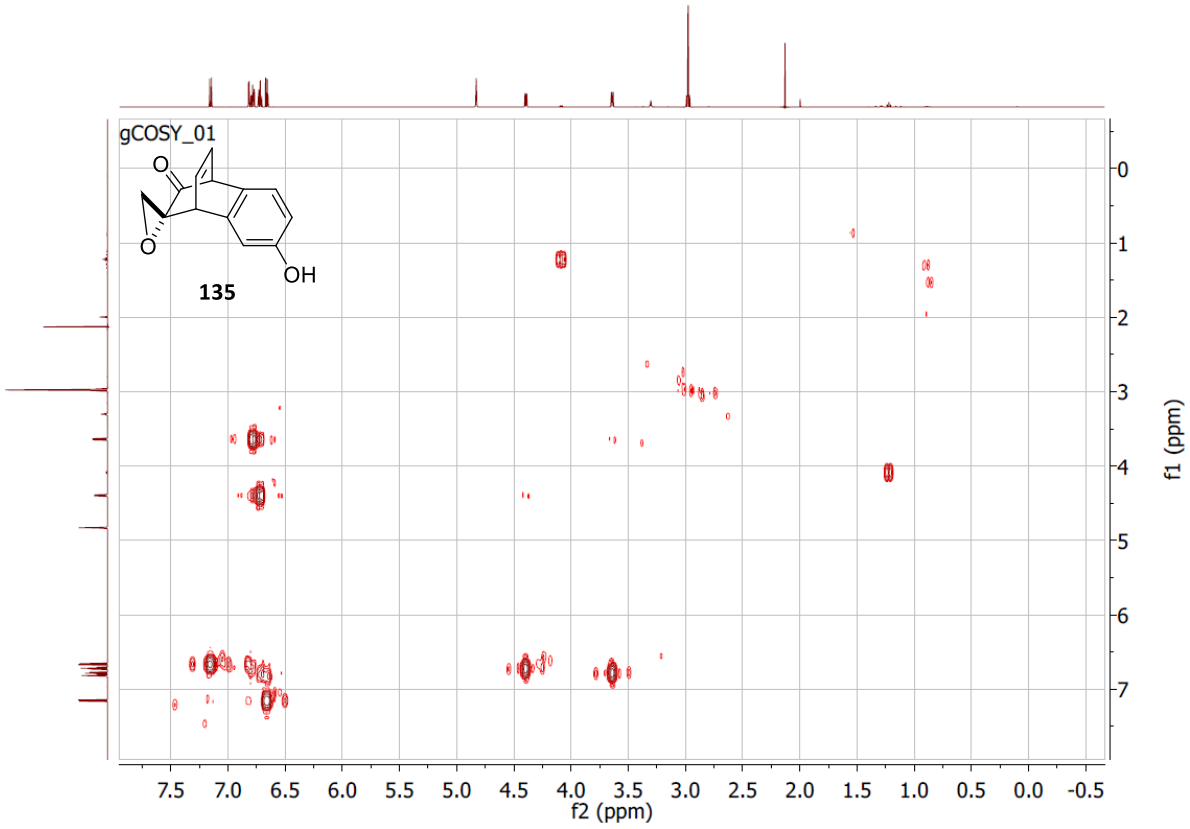
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
287.0564	1	C 12 H 3 N 10	46.93	287.0548	-1.7	-5.8	4.4	16.5	even	ok
	2	C 15 H 11 O 6	100.00	287.0561	-0.3	-1.1	5.0	10.5	even	ok
	3	C 11 H 7 N 6 O 4	13.74	287.0534	-3.0	-10.4	11.0	11.5	even	ok
	4	C 16 H 7 N 4 O 2	56.26	287.0574	1.0	3.6	16.2	15.5	even	ok

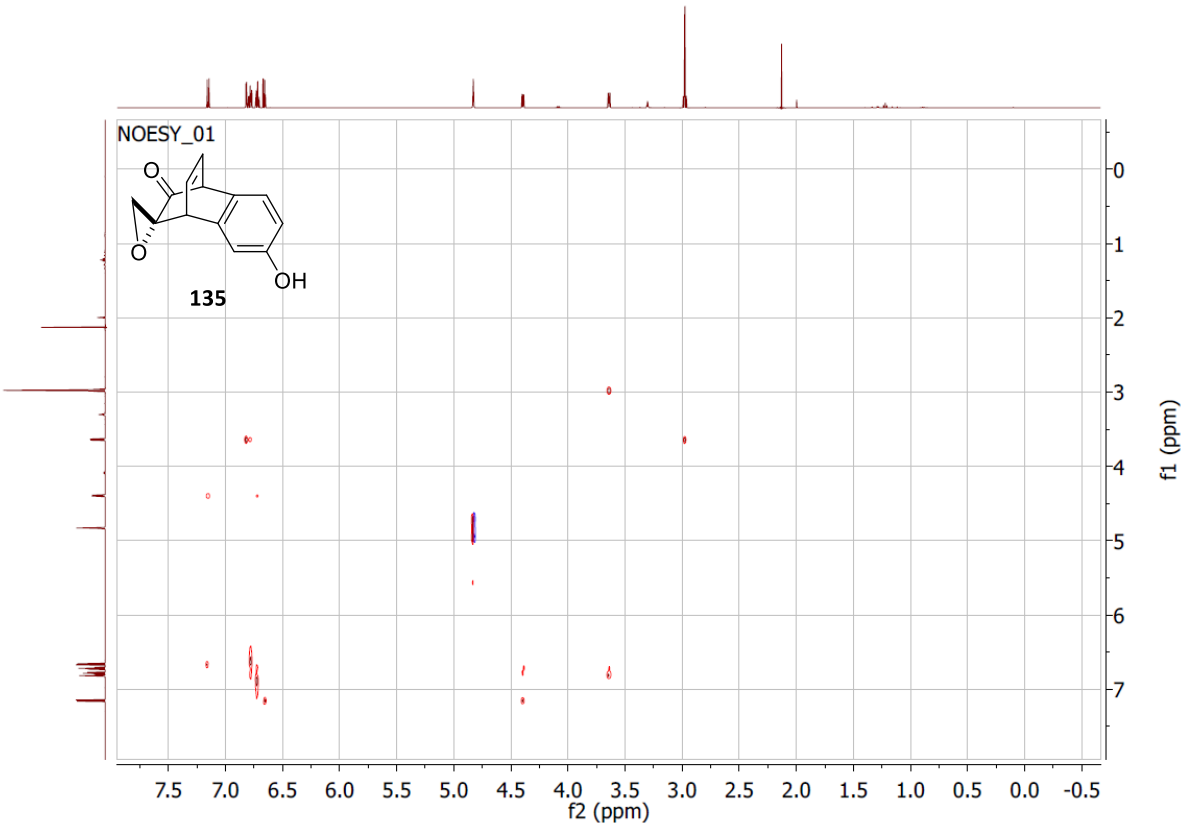

PROTON_01
135
H (d)
6.82
J(2.36)
F (ddd)
6.72
J(7.65, 5.96, 1.77)
B (ddd)
4.40
J(6.01, 1.62, 0.47)
C (d)
2.98
J(5.95)
E (dd)
6.67
J(8.15, 2.46)
A (dd)
3.65
J(6.23, 1.77)
G (ddd)
6.79
J(7.75, 6.22, 1.61)
D (d)
2.98
J(6.01)
I (d)
7.16
J(8.10)
f1 (ppm)

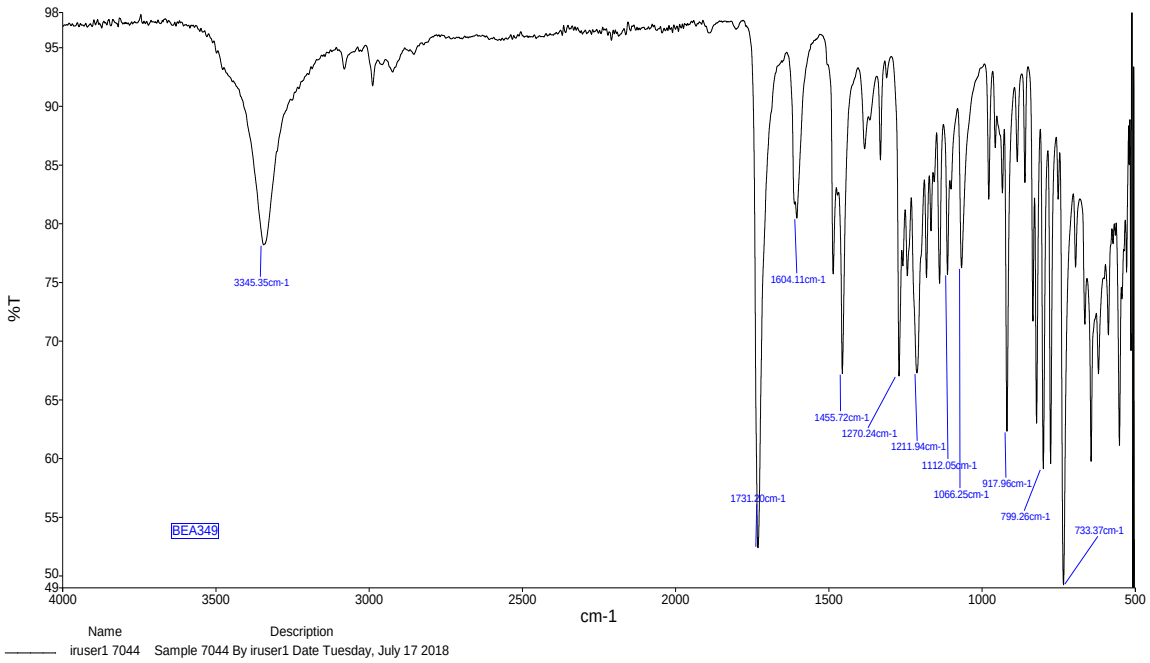

CARBON_01
135
f1 (ppm)


gHMBCAD_01
O
O
OH
135
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f2 (ppm)
0
20
40
60
80
100
120
140
160
180
200
220
f1 (ppm)


gHSQCAD_01
O
O
OH
135
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f2 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
f1 (ppm)


gCOSY_01
O
O
OH
135
f2 (ppm)
f1 (ppm)

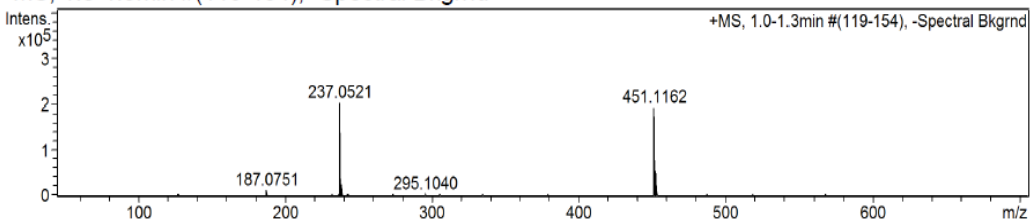

NOESY_01
O
O
OH
135
f2 (ppm)
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_BEA349	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA349_358364_45_01_64743.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	14/08/2018 11:42:12
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	127.0881	3397	1.7	68	1457.2
2	187.0751	12673	6.2	414	1798.9
3	236.0763	4001	2.0	90	163.3
4	237.0521	203135	100.0	8609	8153.1
5	238.0564	23460	11.5	931	925.5
6	295.1040	4550	2.2	140	361.4
7	451.1162	192247	94.6	16339	6404.8
8	452.1194	54787	27.0	4380	1788.4
9	453.1225	9726	4.8	781	311.1
10	487.0950	3692	1.8	339	146.8

Generate Molecular Formula Parameters

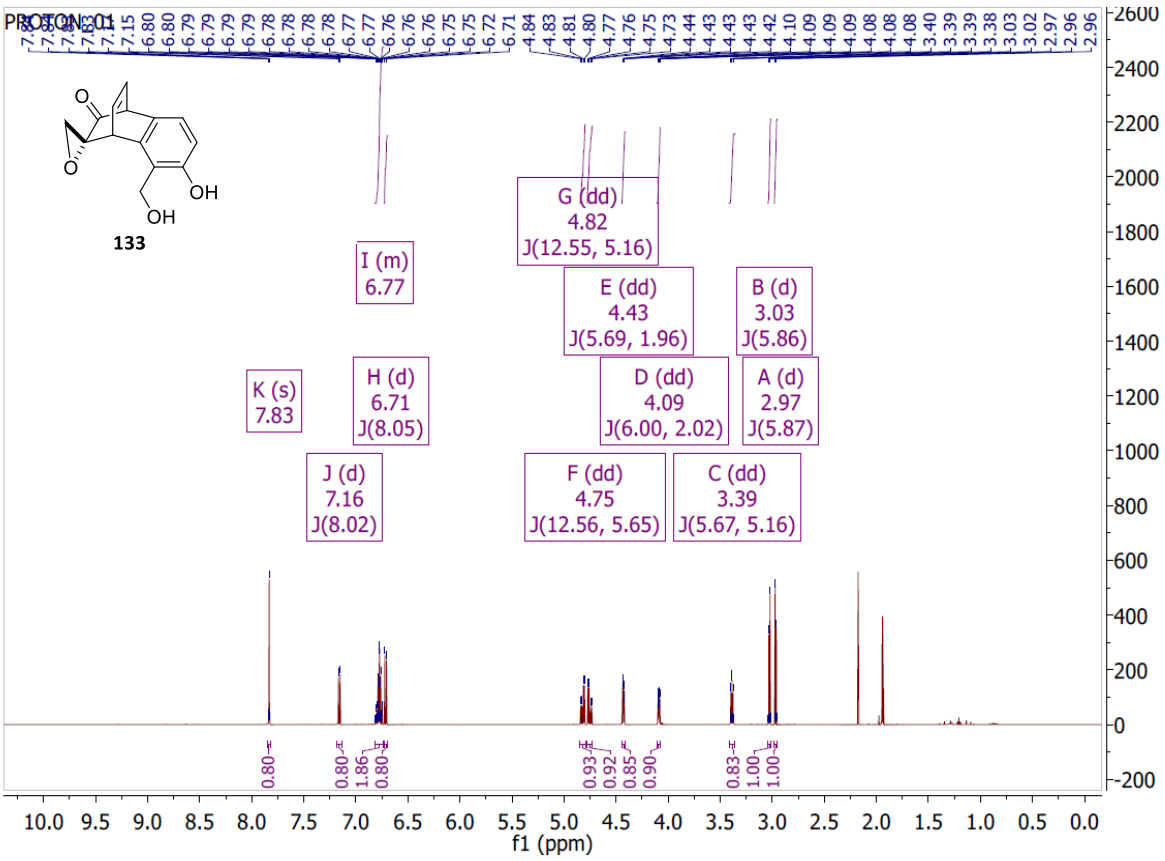
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

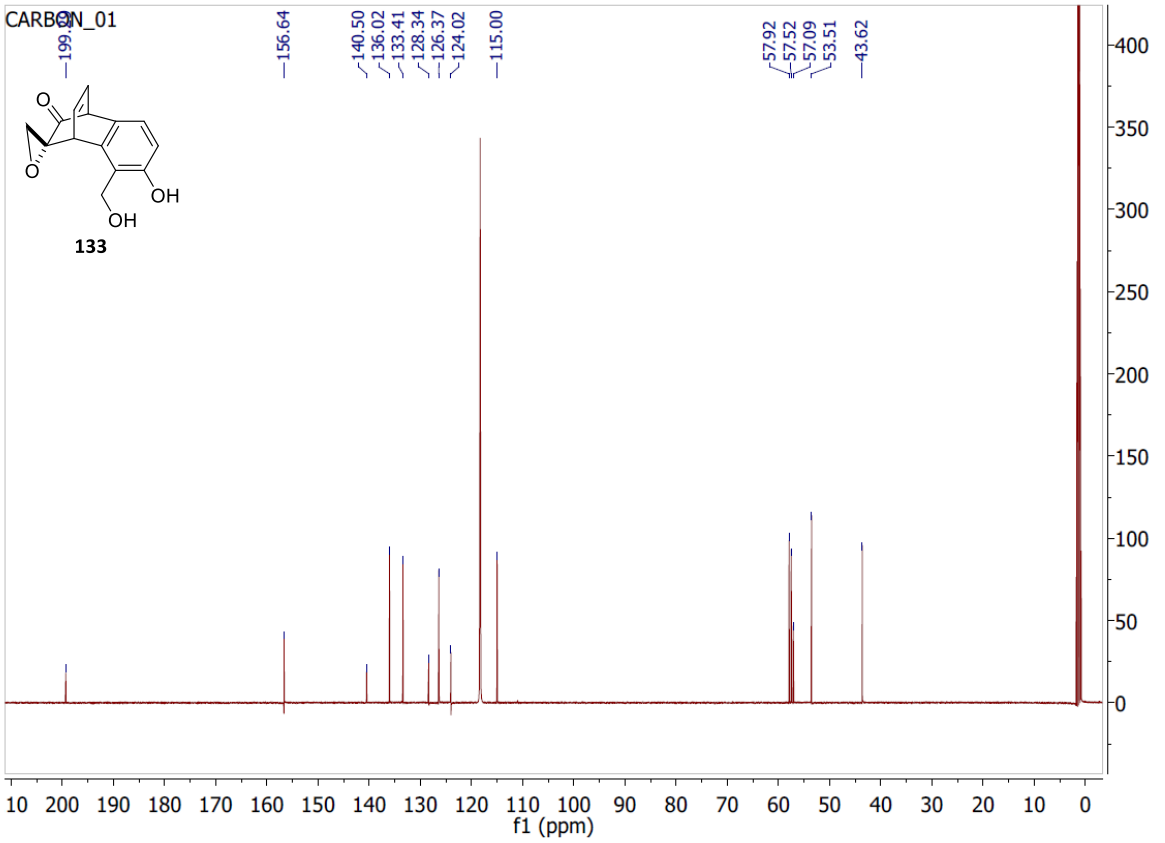
Expected Formula C13 H10 O3 **Adduct(s):** H, Na

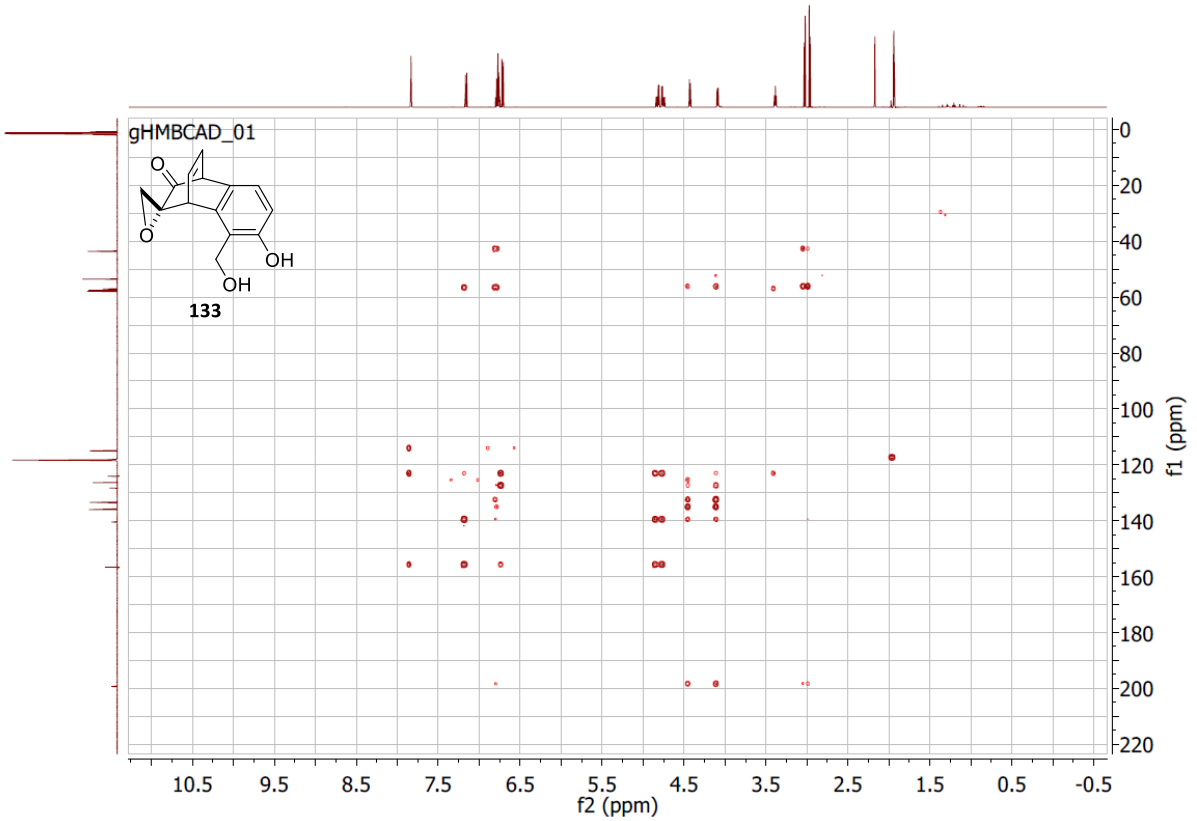
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	237.0521	237.0522	-0.50	0.0154	C 13 H 10 Na 1 O 3

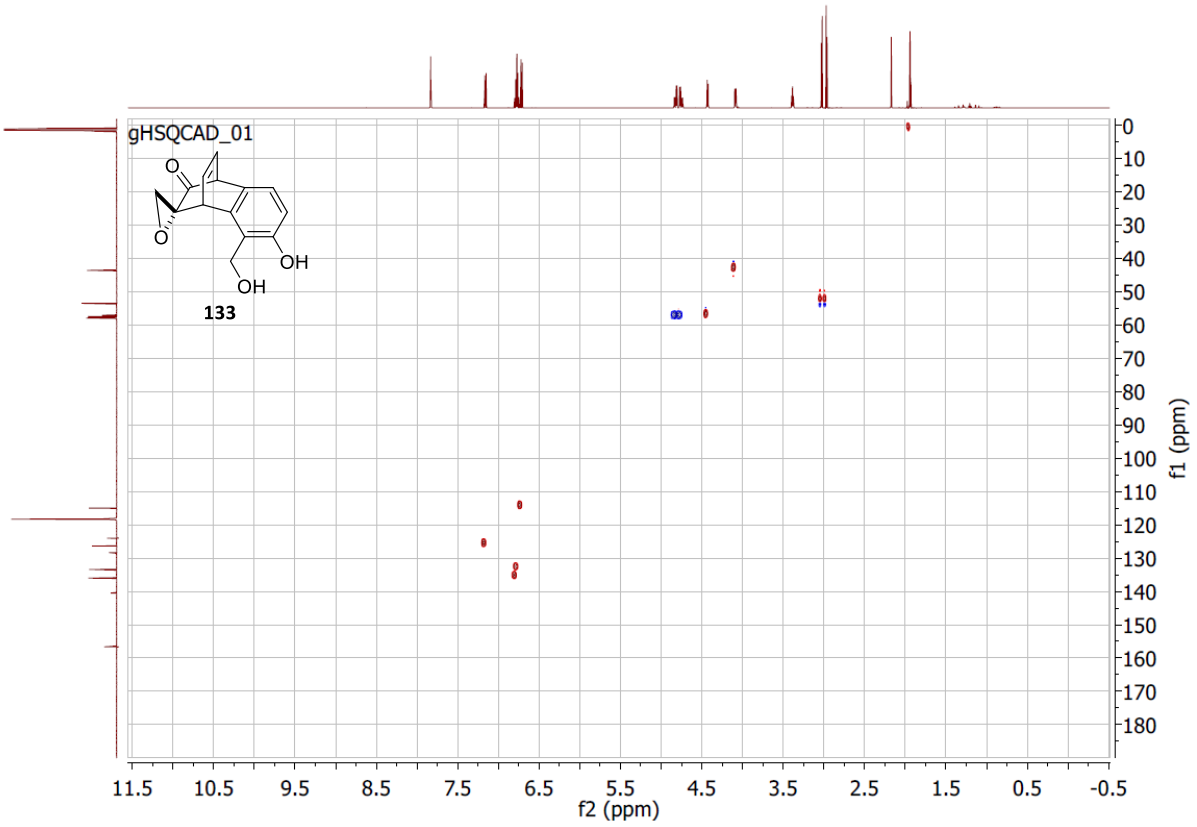
Note: Sigma fits < 0.05 indicates high probability of correct MF.

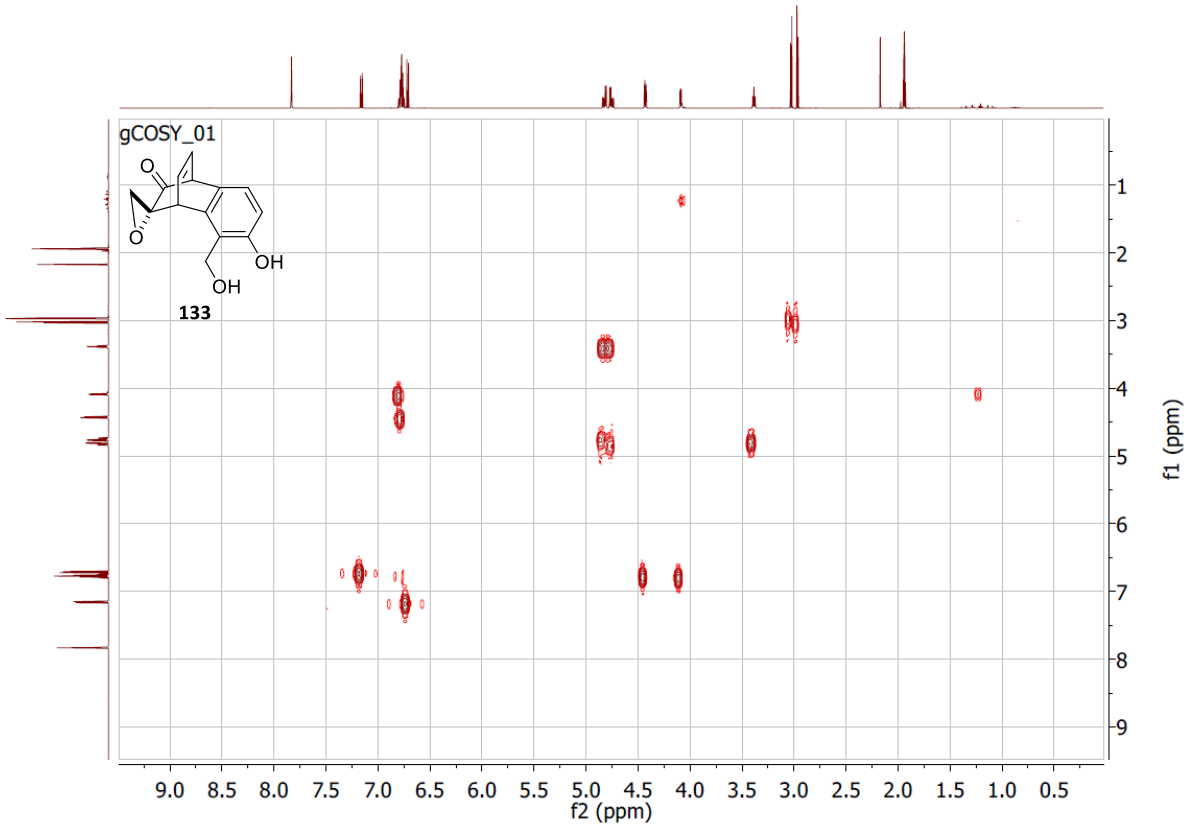
For formula confirmation the mass error / accuracy at 200 Da should be better than 25 ppm, for 500 Da better than 10 ppm and for 1000 Da better than 5 ppm

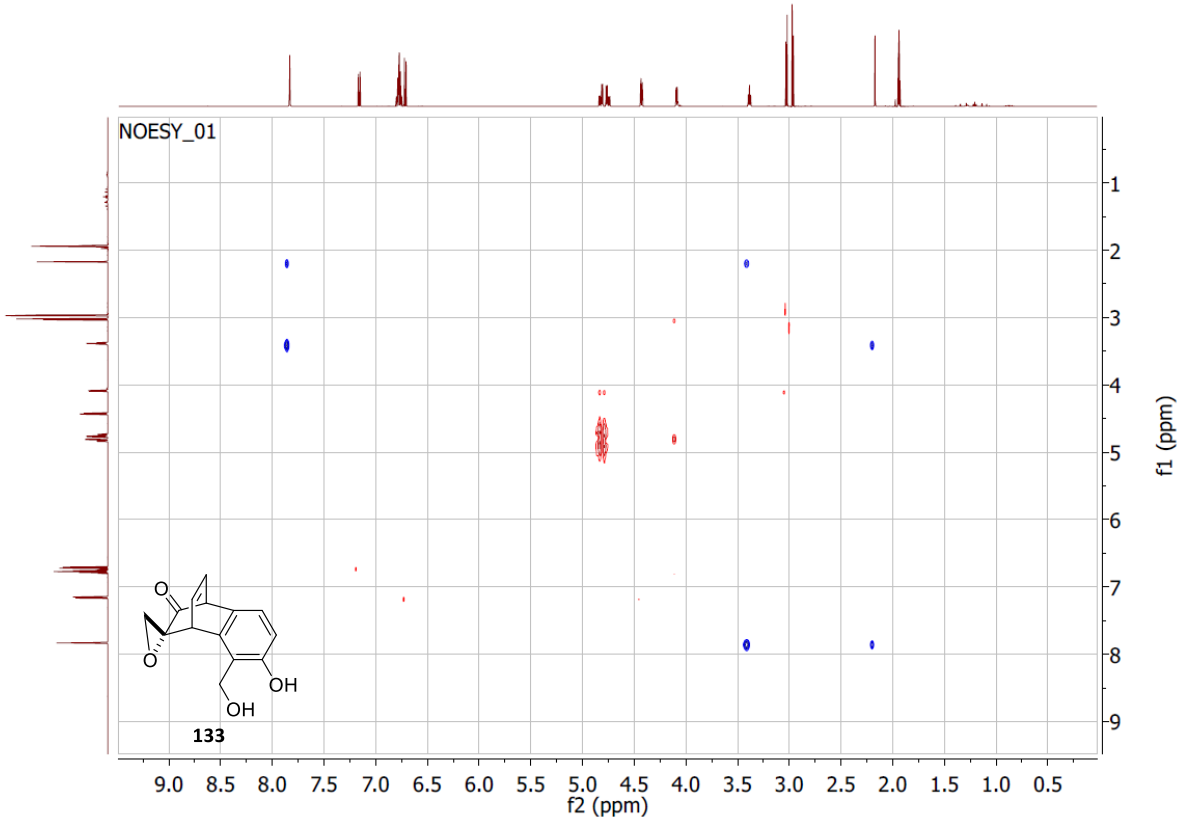

PROTON_01
O
O
OH
OH
133
G (dd)
4.82
J(12.55, 5.16)
I (m)
6.77
E (dd)
4.43
J(5.69, 1.96)
B (d)
3.03
J(5.86)
K (s)
7.83
H (d)
6.71
J(8.05)
D (dd)
4.09
J(6.00, 2.02)
A (d)
2.97
J(5.87)
J (d)
7.16
J(8.02)
F (dd)
4.75
J(12.56, 5.65)
C (dd)
3.39
J(5.67, 5.16)
0.80
0.80
1.86
0.80
0.93
0.92
0.85
0.90
0.83
1.00
1.00
f1 (ppm)

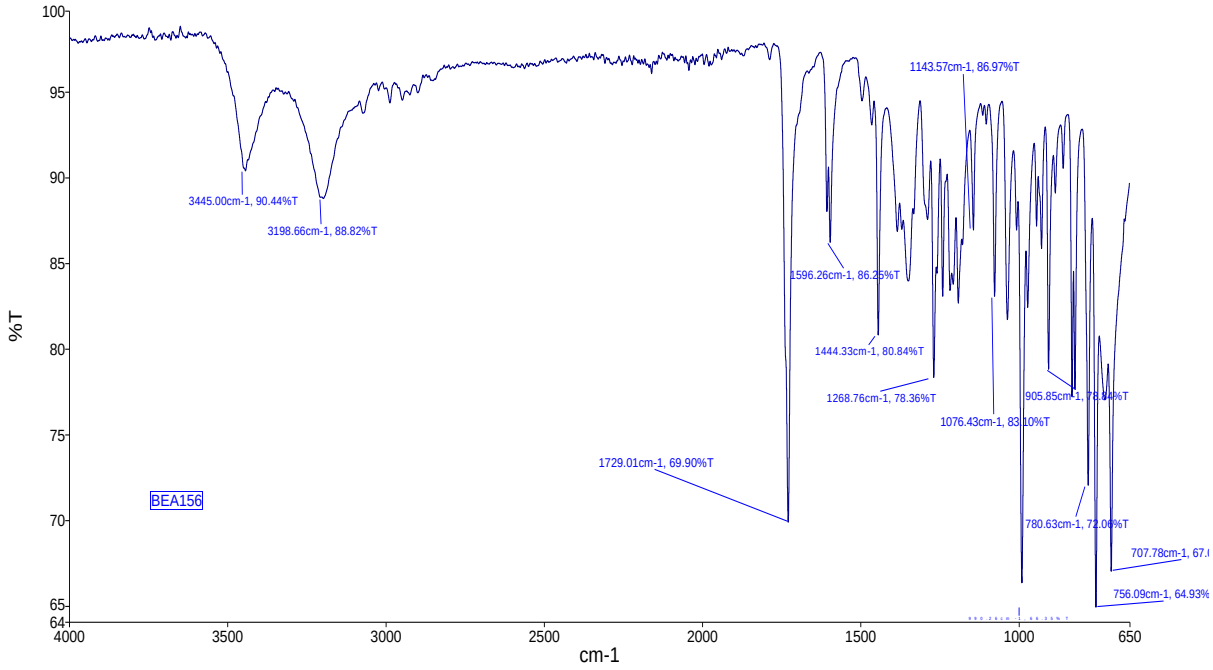

CARBON_01
199.
156.64
140.50
136.02
133.41
128.34
126.37
124.02
115.00
57.92
57.52
57.09
53.51
43.62
O
O
OH
OH
133
f1 (ppm)


gHMBCAD_01
O
O
OH
OH
133
0
20
40
60
80
100
120
140
160
180
200
220
f1 (ppm)
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f2 (ppm)


gHSQCAD_01
O
O
OH
OH
133
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
f1 (ppm)
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f2 (ppm)


gCOSY_01
O
O
OH
OH
133
f1 (ppm)
f2 (ppm)

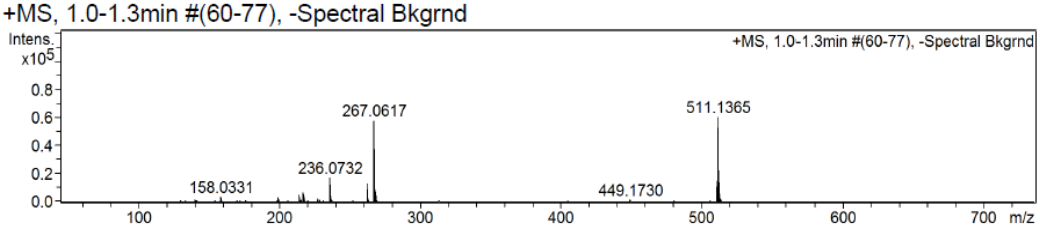

NOESY_01
O
O
OH
OH
133
f1 (ppm)
f2 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_BEA156 C	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA156 C_349496_72_01_54605.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	28/10/2016 10:16:57
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	158.0331	3424	5.7	50	1926.9
2	199.0745	3197	5.3	111	640.2
3	214.1018	5130	8.5	120	773.7
4	217.0845	6870	11.4	277	977.9
5	236.0732	17062	28.3	370	1788.0
6	262.1056	13123	21.8	714	1405.5
7	267.0617	57830	95.9	2837	7041.7
8	268.0649	7594	12.6	404	951.0
9	511.1365	60332	100.0	5259	10493.2
10	512.1383	16337	27.1	1634	2764.4

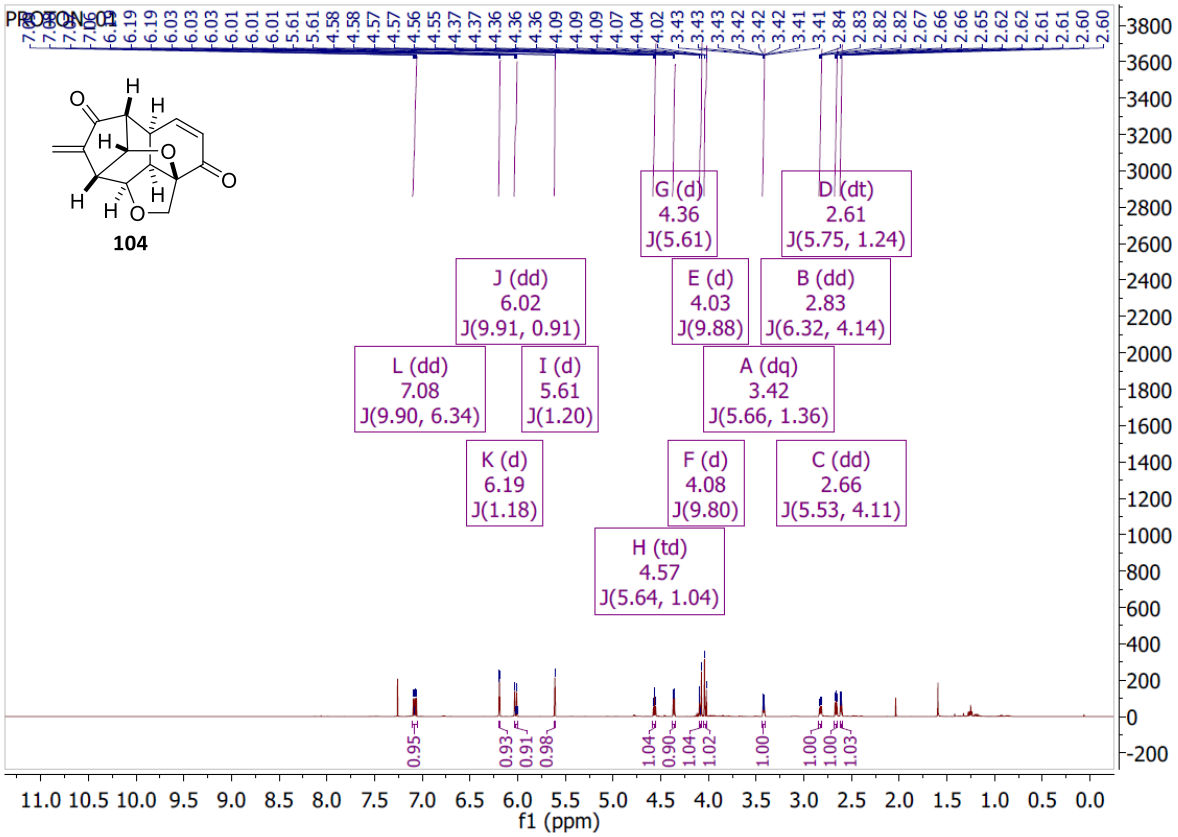
Generate Molecular Formula Parameters

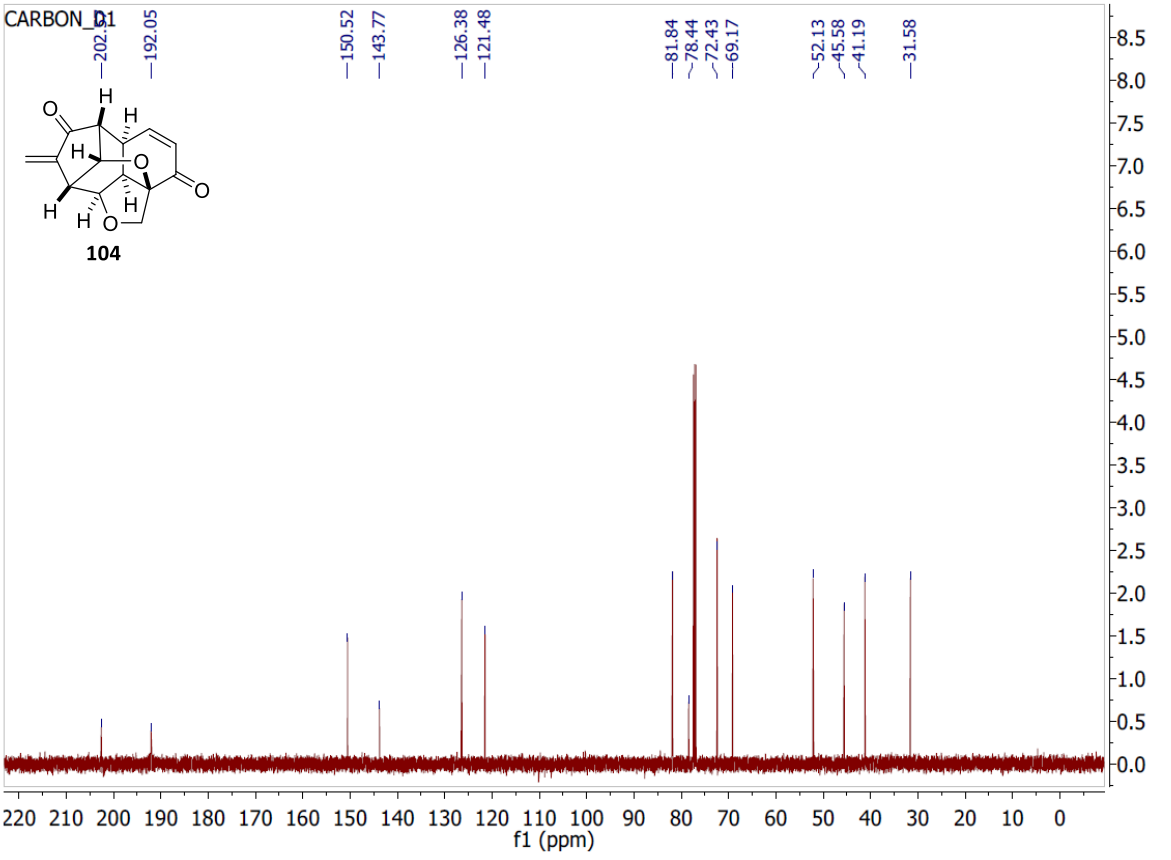
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

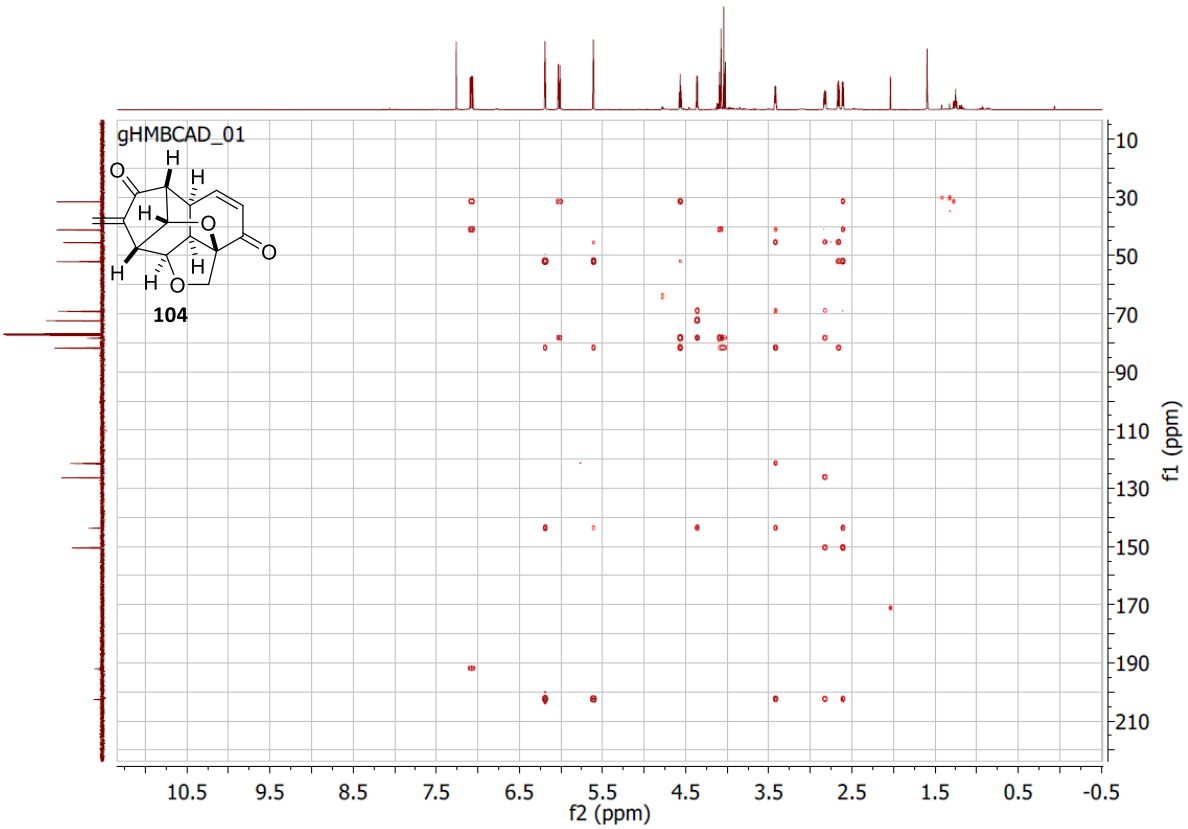
Expected Formula C14 H12 O4 **Adduct(s):** H, Na

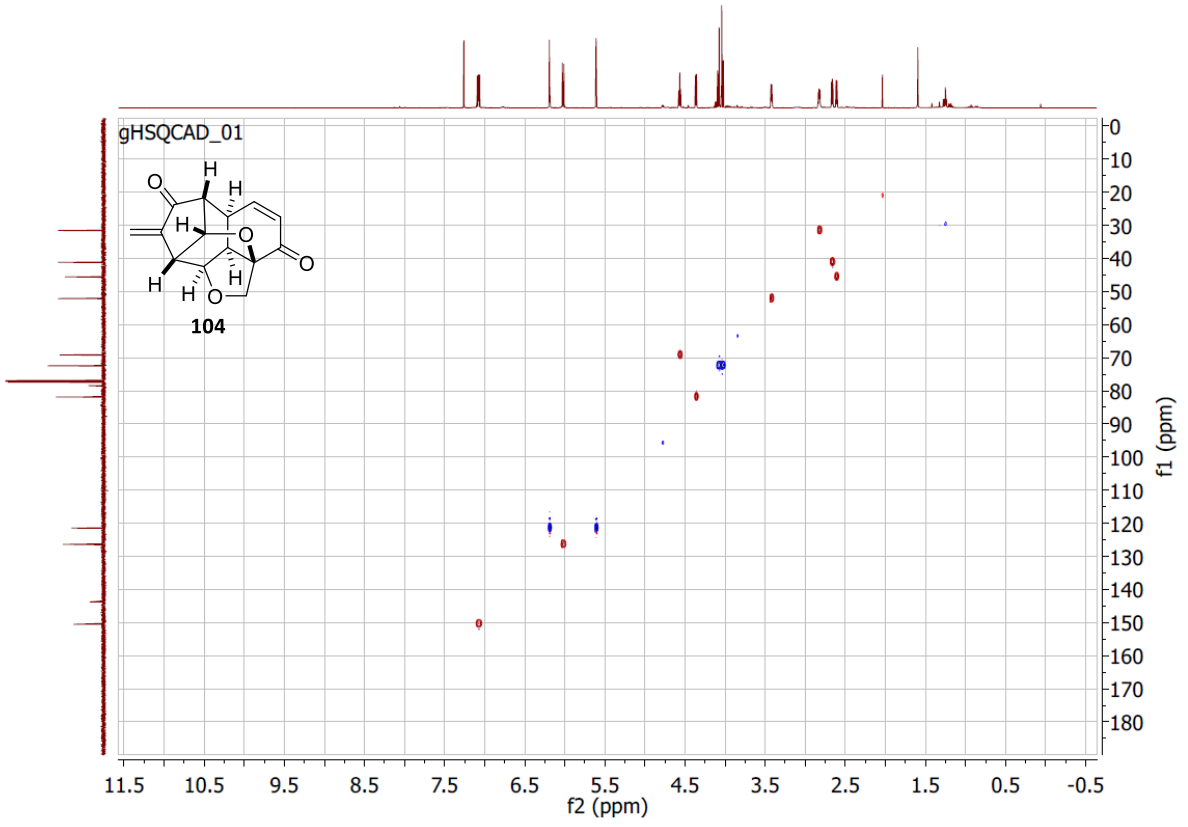
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	267.0617	267.063329	3.90	0.0123	C 14 H 12 Na 1 O 4

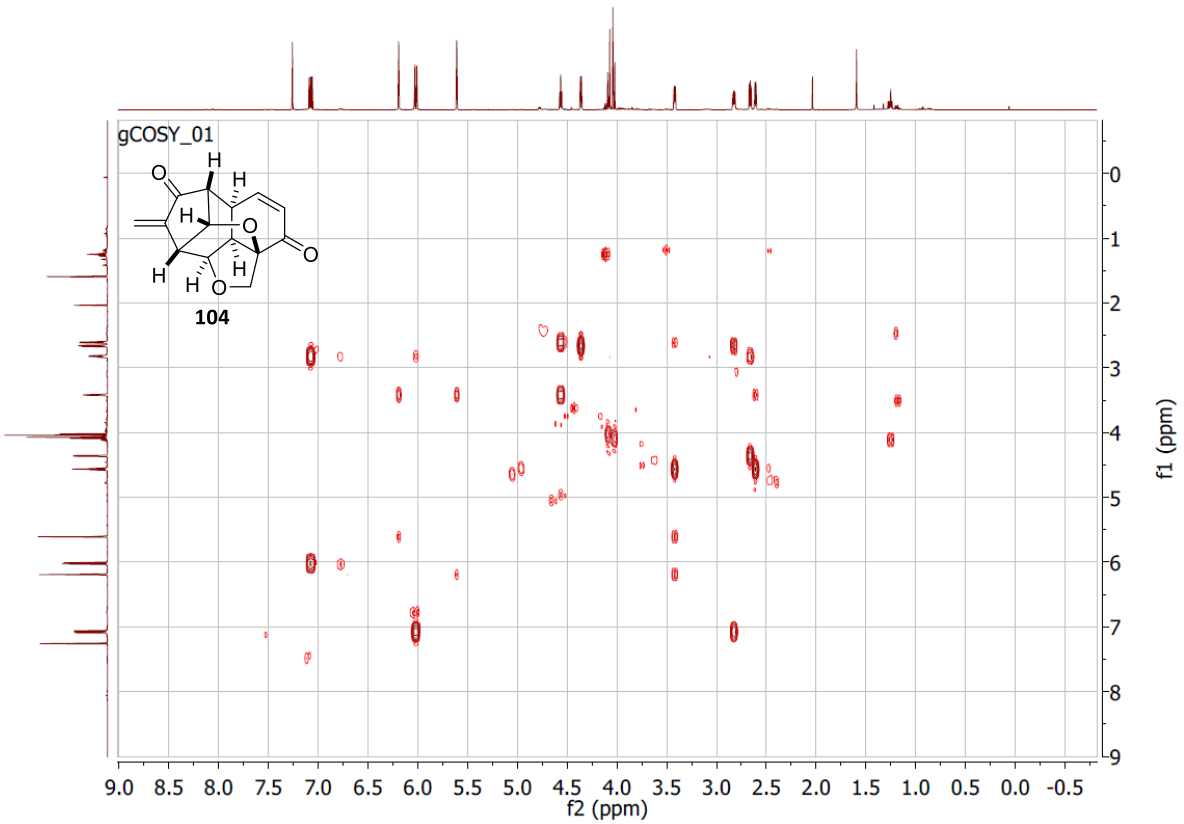
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

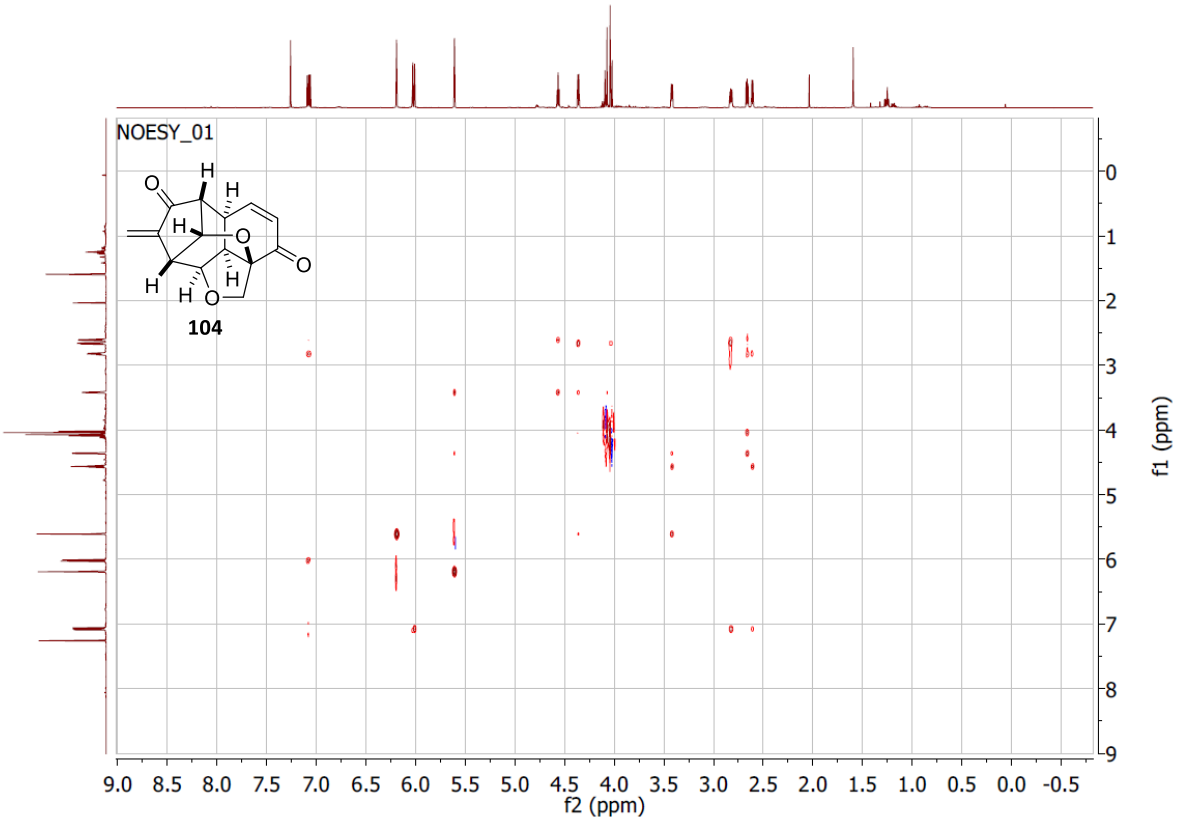

PROTON_01
104
G (d)
4.36
J(5.61)
D (dt)
2.61
J(5.75, 1.24)
J (dd)
6.02
J(9.91, 0.91)
E (d)
4.03
J(9.88)
B (dd)
2.83
J(6.32, 4.14)
L (dd)
7.08
J(9.90, 6.34)
I (d)
5.61
J(1.20)
A (dq)
3.42
J(5.66, 1.36)
K (d)
6.19
J(1.18)
F (d)
4.08
J(9.80)
C (dd)
2.66
J(5.53, 4.11)
H (td)
4.57
J(5.64, 1.04)
f1 (ppm)

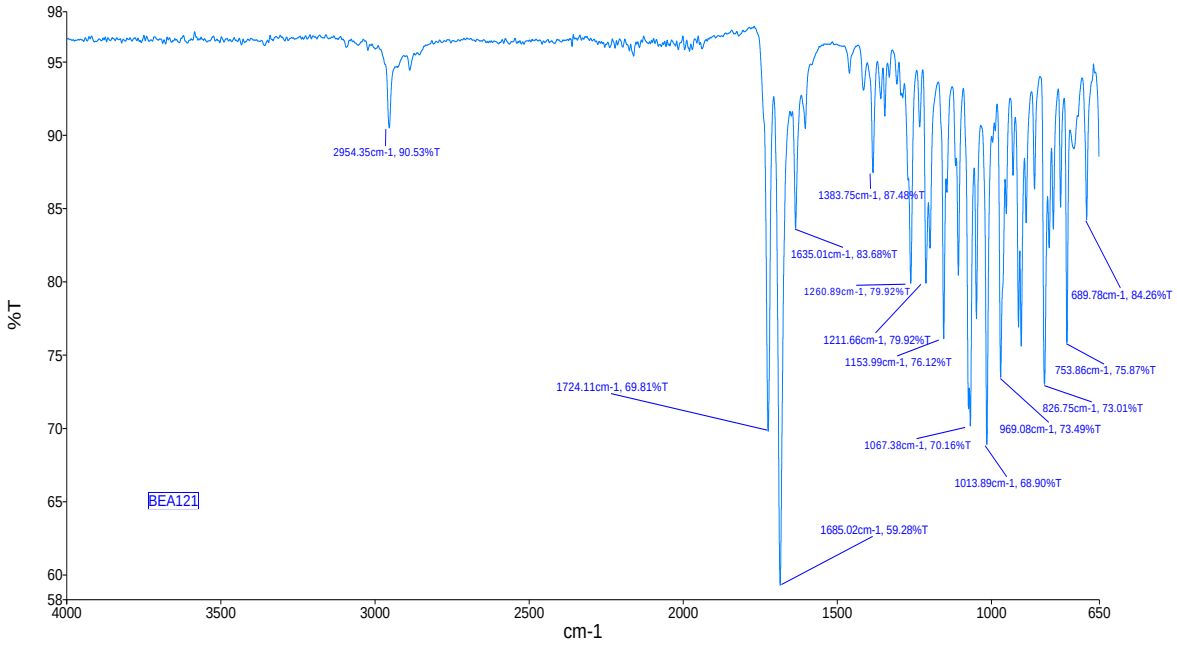

CARBON_01
104
f1 (ppm)


gHMBCAD_01
104
f2 (ppm)
f1 (ppm)


gHSQCAD_01
104
f2 (ppm)
f1 (ppm)


gCOSY_01
104
f2 (ppm)
f1 (ppm)


NOESY_01
104
f2 (ppm)
f1 (ppm)



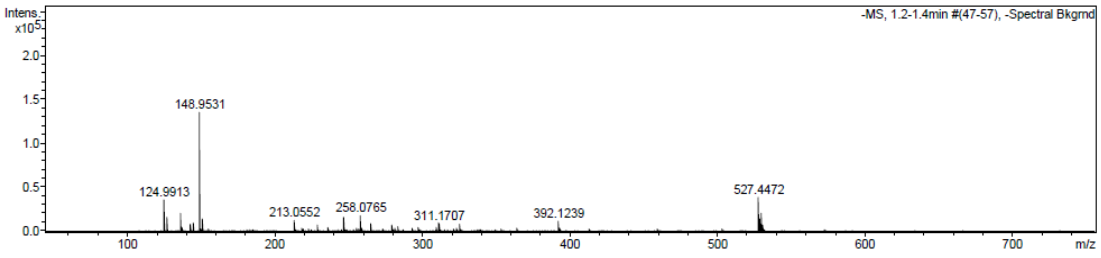
Mass Spectrum SmartFormula Report

Analysis Info

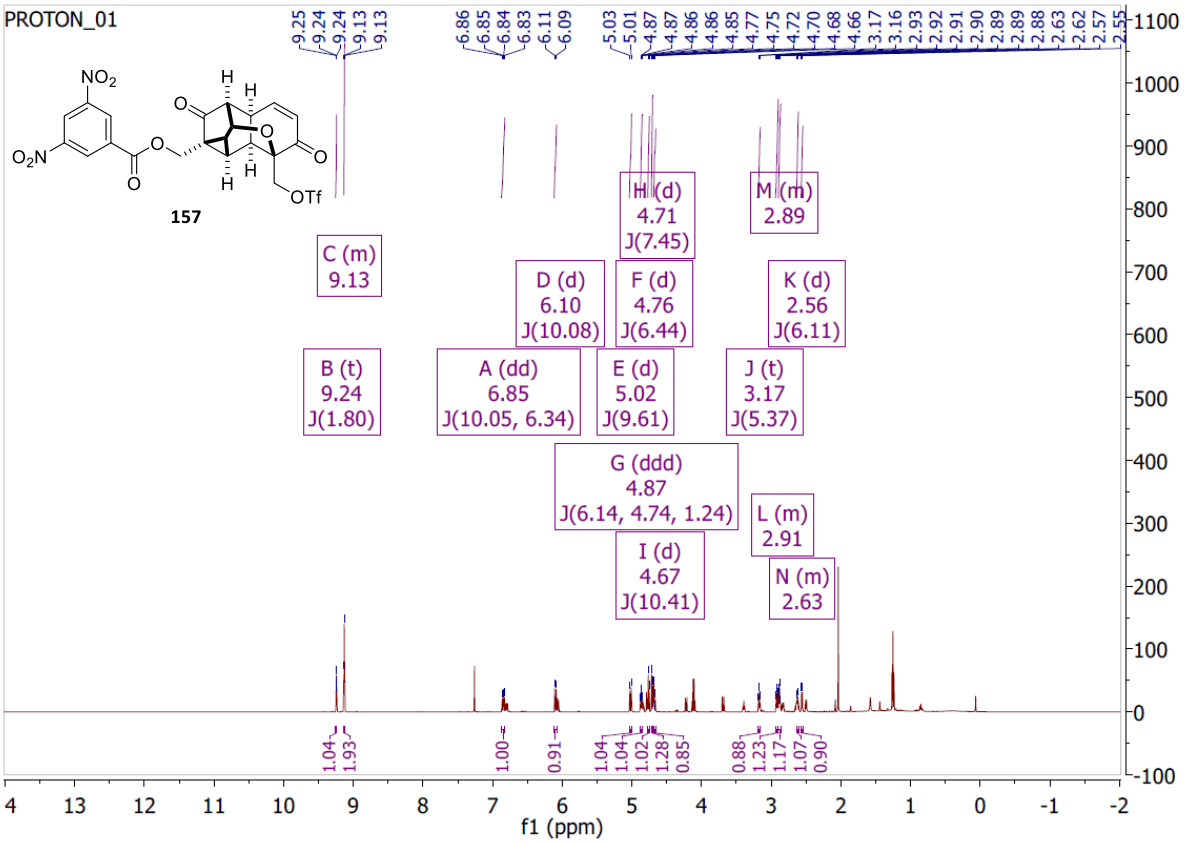
Analysis Name	Z:\ba_sel_BEA311_358363_44_01_64735.d	Acquisition Date	8/14/2018 11:05:03 AM
Method	Confirm Formula Negative 50to500 loop inj.m		
Sample Name	ba_sel_BEA311_358363	Operator	admin
Comment		Instrument / Ser#	micrOTOF 161

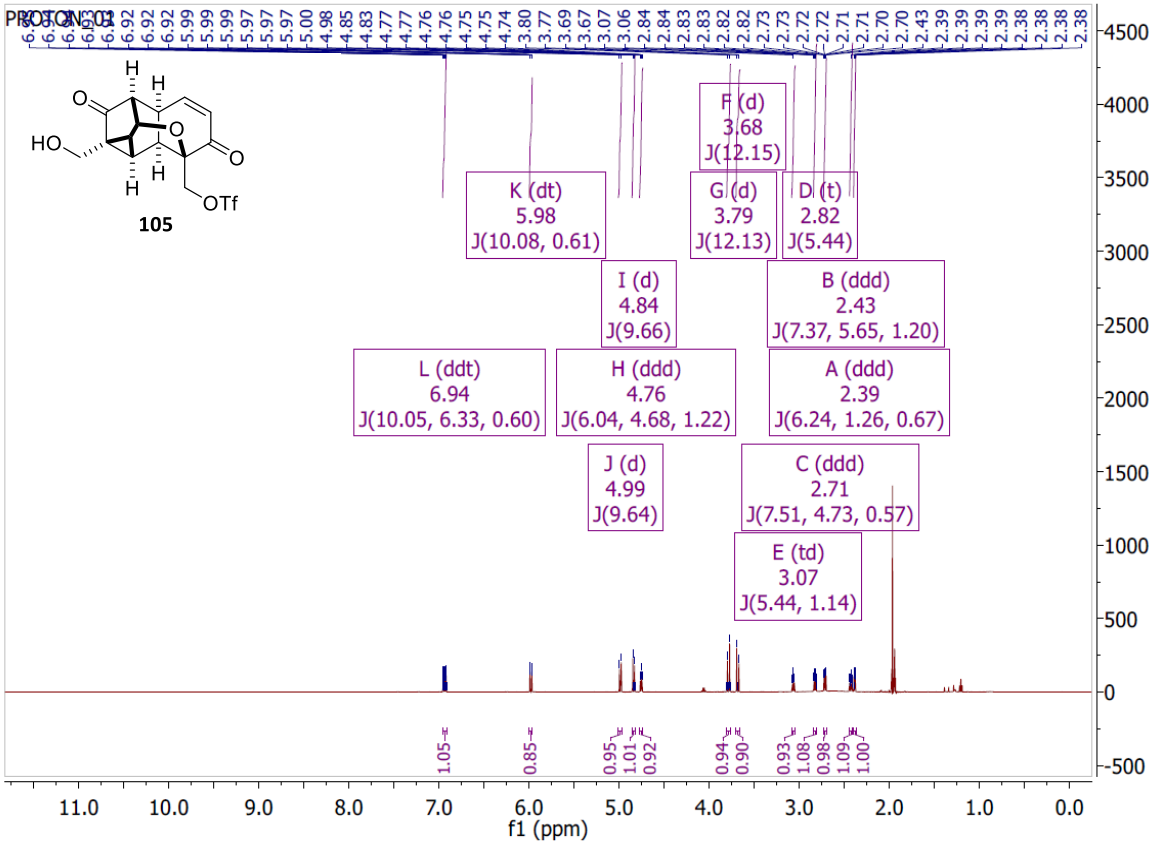
Acquisition Parameter

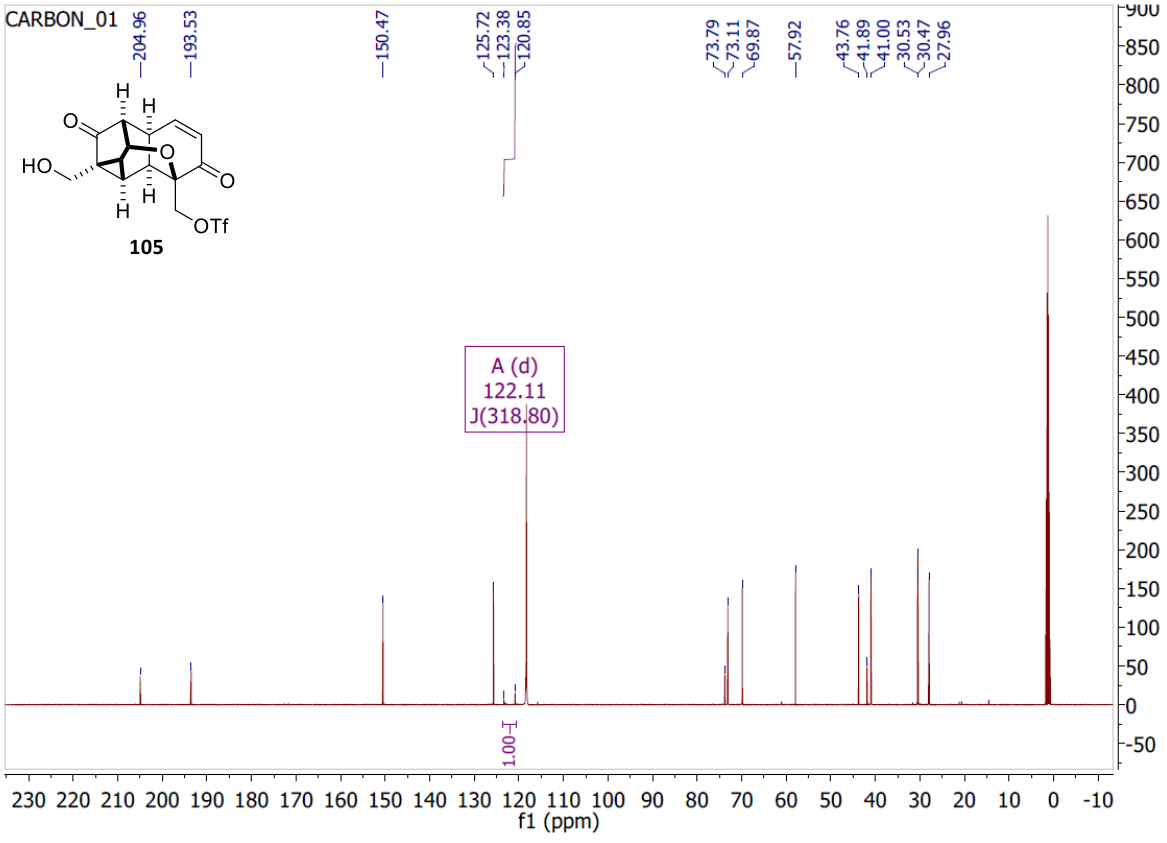
Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.2 Bar
Focus	Not active			Set Dry Heater	220 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.2 l/min
Scan End	750 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

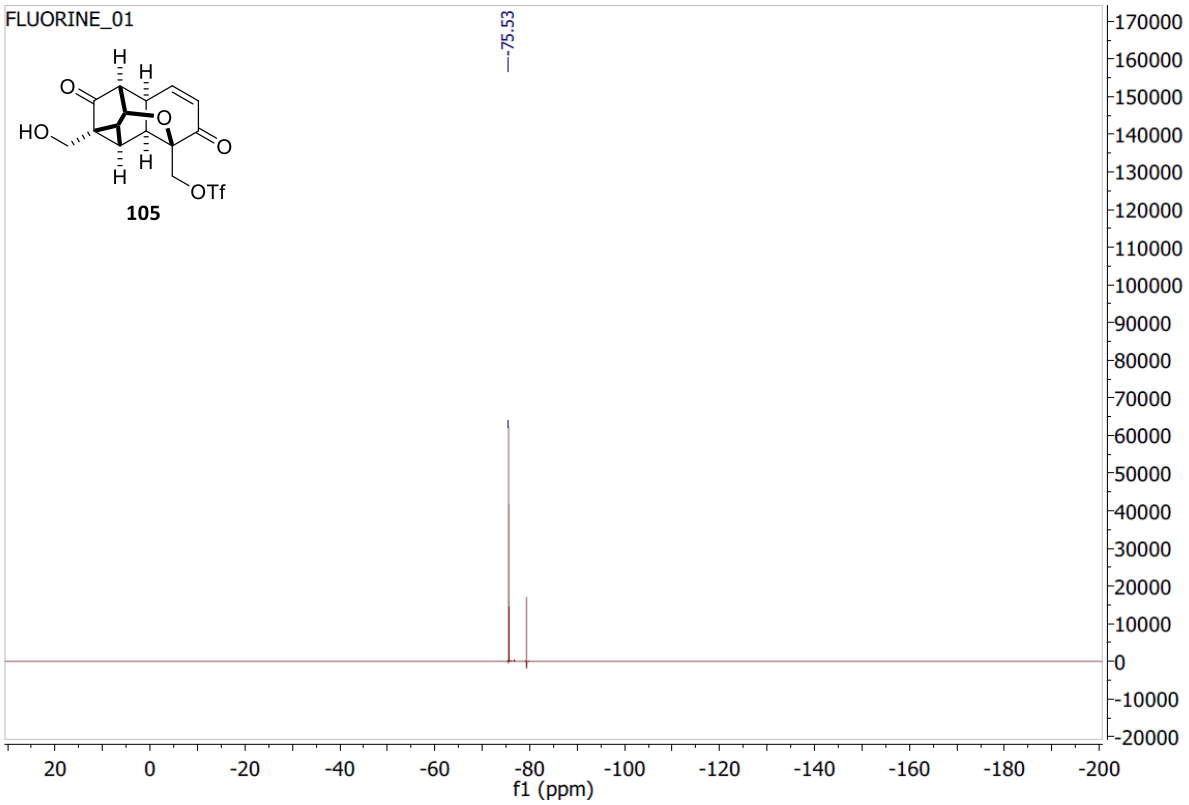


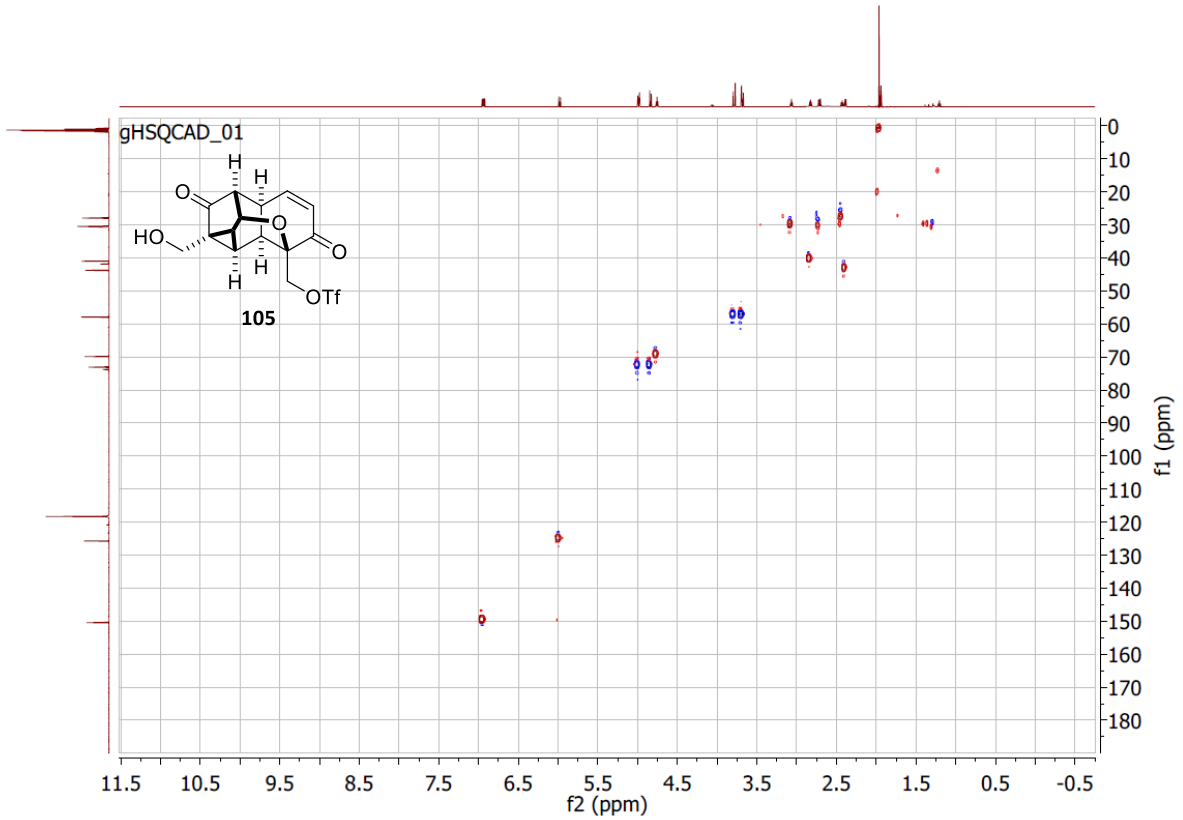
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
243.0678	1	C 14 H 11 O 4	98.75	243.0663	-1.5	-6.2	573.2	9.5	even	ok
	2	C 15 H 7 N 4	100.00	243.0676	-0.2	-0.7	576.3	14.5	even	ok

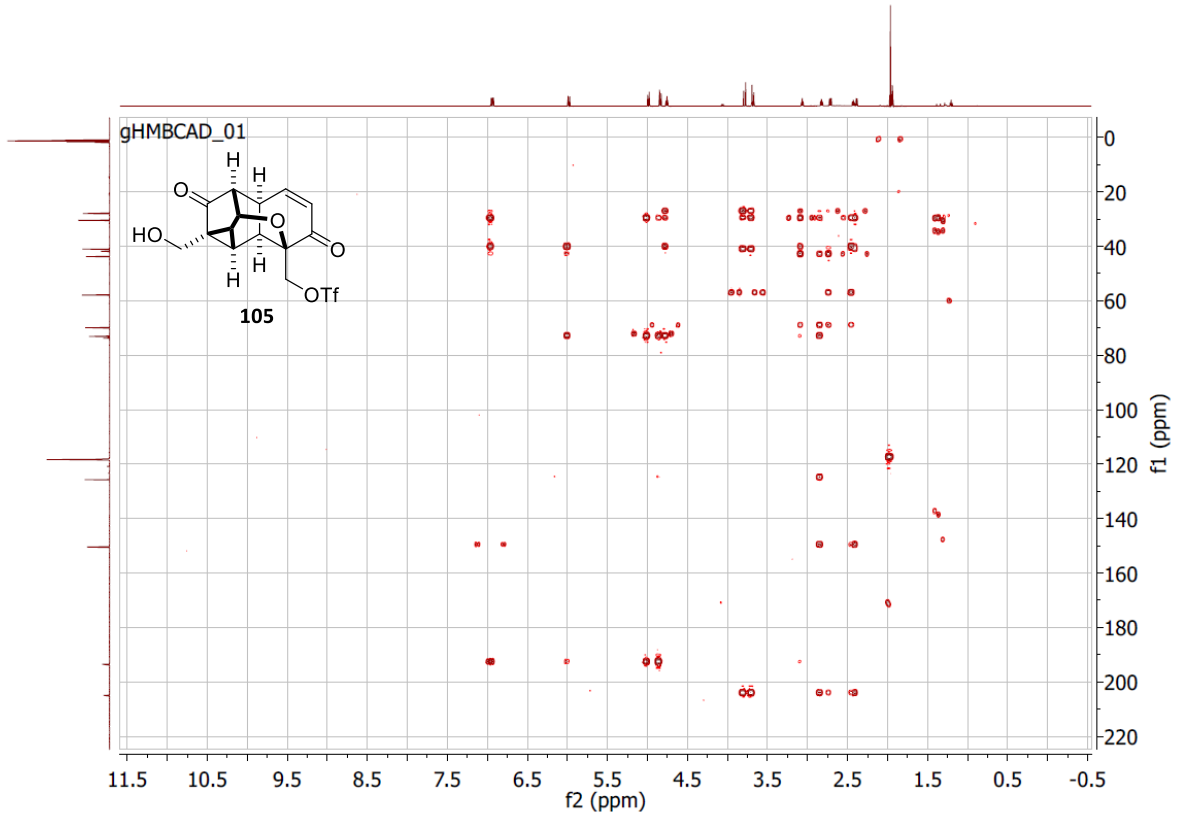

PROTON_01
157
C (m)
9.13
B (t)
9.24
J(1.80)
D (d)
6.10
J(10.08)
A (dd)
6.85
J(10.05, 6.34)
H (d)
4.71
J(7.45)
F (d)
4.76
J(6.44)
E (d)
5.02
J(9.61)
G (ddd)
4.87
J(6.14, 4.74, 1.24)
I (d)
4.67
J(10.41)
M (m)
2.89
K (d)
2.56
J(6.11)
J (t)
3.17
J(5.37)
L (m)
2.91
N (m)
2.63
f1 (ppm)

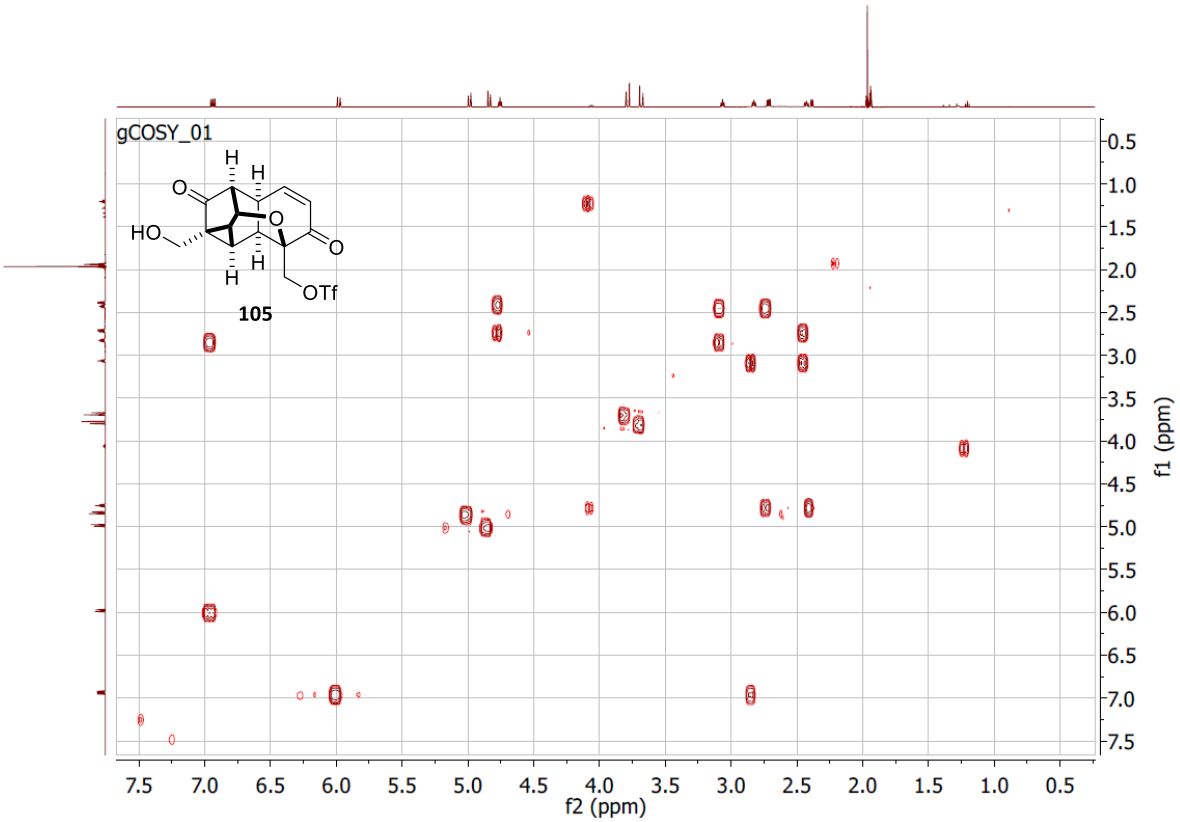

PROTON_01
105
K (dt)
5.98
J(10.08, 0.61)
F (d)
3.68
J(12.15)
G (d)
3.79
J(12.13)
D (t)
2.82
J(5.44)
I (d)
4.84
J(9.66)
B (ddd)
2.43
J(7.37, 5.65, 1.20)
L (ddt)
6.94
J(10.05, 6.33, 0.60)
H (ddd)
4.76
J(6.04, 4.68, 1.22)
A (ddd)
2.39
J(6.24, 1.26, 0.67)
J (d)
4.99
J(9.64)
C (ddd)
2.71
J(7.51, 4.73, 0.57)
E (td)
3.07
J(5.44, 1.14)
f1 (ppm)

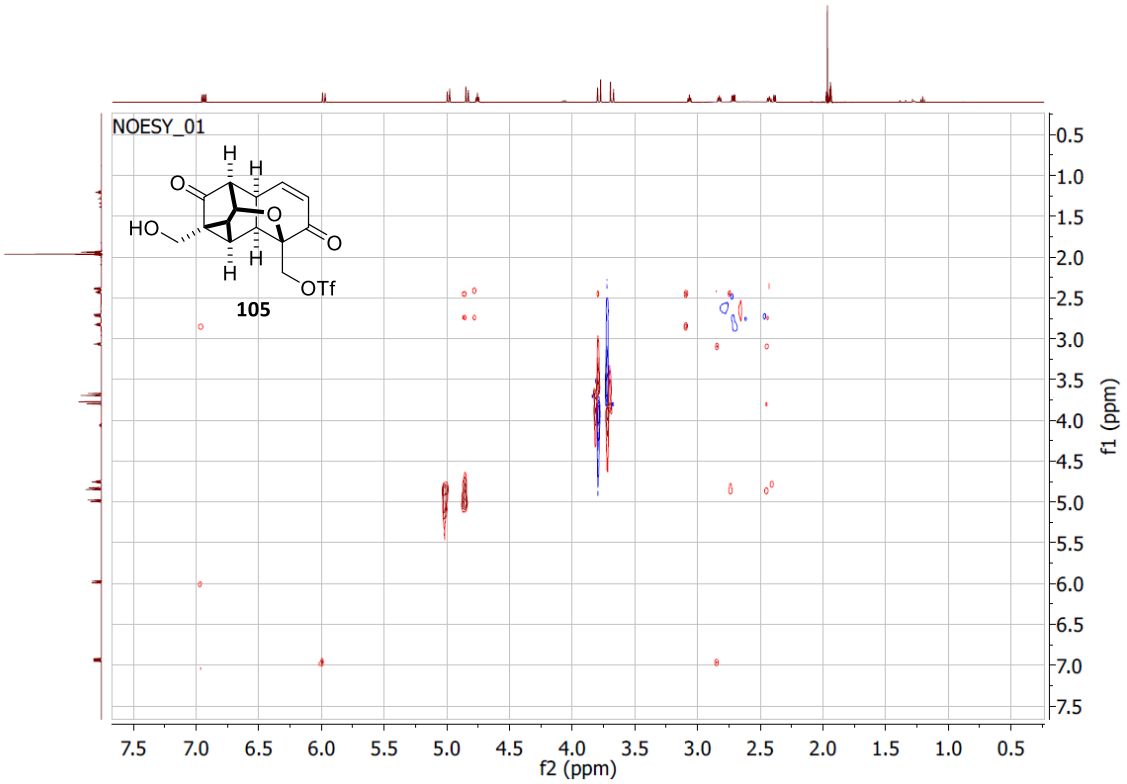

CARBON_01
105
A (d)
122.11
J(318.80)
f1 (ppm)

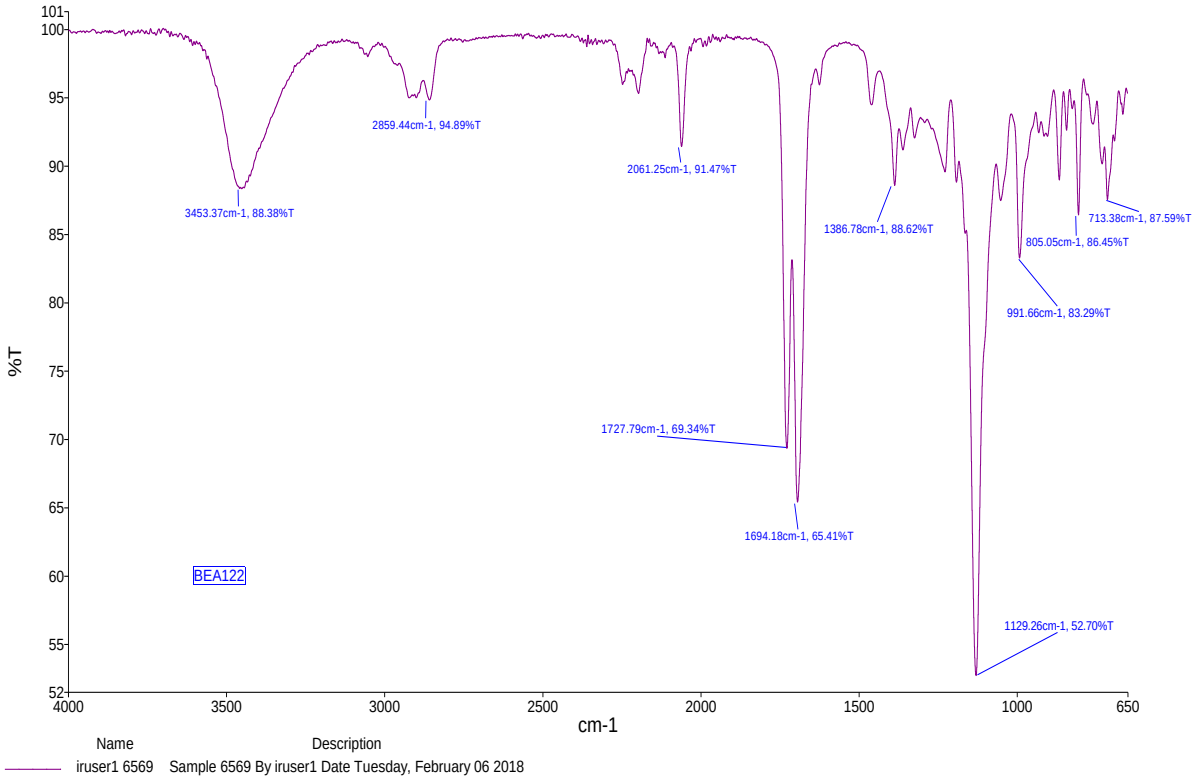

FLUORINE_01
-75.53
105
f1 (ppm)


gHSQCAD_01
105
f2 (ppm)
f1 (ppm)


gHMBCAD_01
HO
OTf
105
f2 (ppm)
f1 (ppm)


gCOSY_01
HO
OTf
105
f2 (ppm)
f1 (ppm)

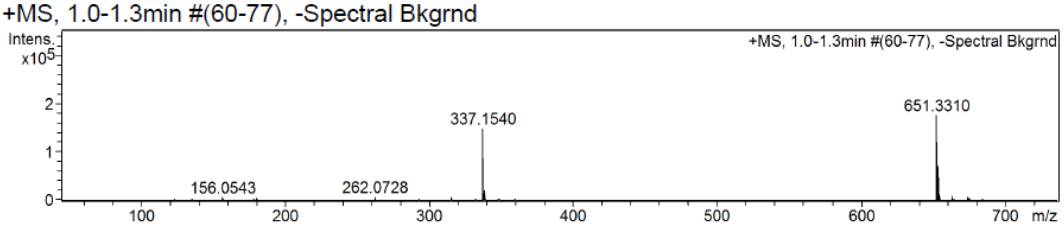

NOESY_01
HO
O
O
O
H
H
H
H
OTf
105
f2 (ppm)
f1 (ppm)


%T
cm-1
3453.37cm-1, 88.38%T
2859.44cm-1, 94.89%T
2061.25cm-1, 91.47%T
1727.79cm-1, 69.34%T
1694.18cm-1, 65.41%T
1386.78cm-1, 88.62%T
1129.26cm-1, 52.70%T
991.66cm-1, 83.29%T
805.05cm-1, 86.45%T
713.38cm-1, 87.59%T
BEA122
Name
Description
iruser1 6569
Sample 6569 By iruser1 Date Tuesday, February 06 2018

Confirmation of Expected Formula

Sample-ID	ba_sel_BEA122 E	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA122 E_347790_67_01_52580.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	20/05/2016 13:04:54
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	156.0543	6742	3.8	116	6418.6
2	262.0728	6820	3.9	353	3180.9
3	315.1738	6235	3.6	399	676.2
4	337.1540	147970	84.4	7884	8975.8
5	338.1572	20756	11.8	1343	1234.2
6	651.3310	175287	100.0	14822	3429.8
7	652.3193	68798	39.2	6696	1307.1
8	653.3232	12389	7.1	1269	228.6
9	662.3156	9524	5.4	1069	139.9
10	673.3001	5721	3.3	1102	90.2

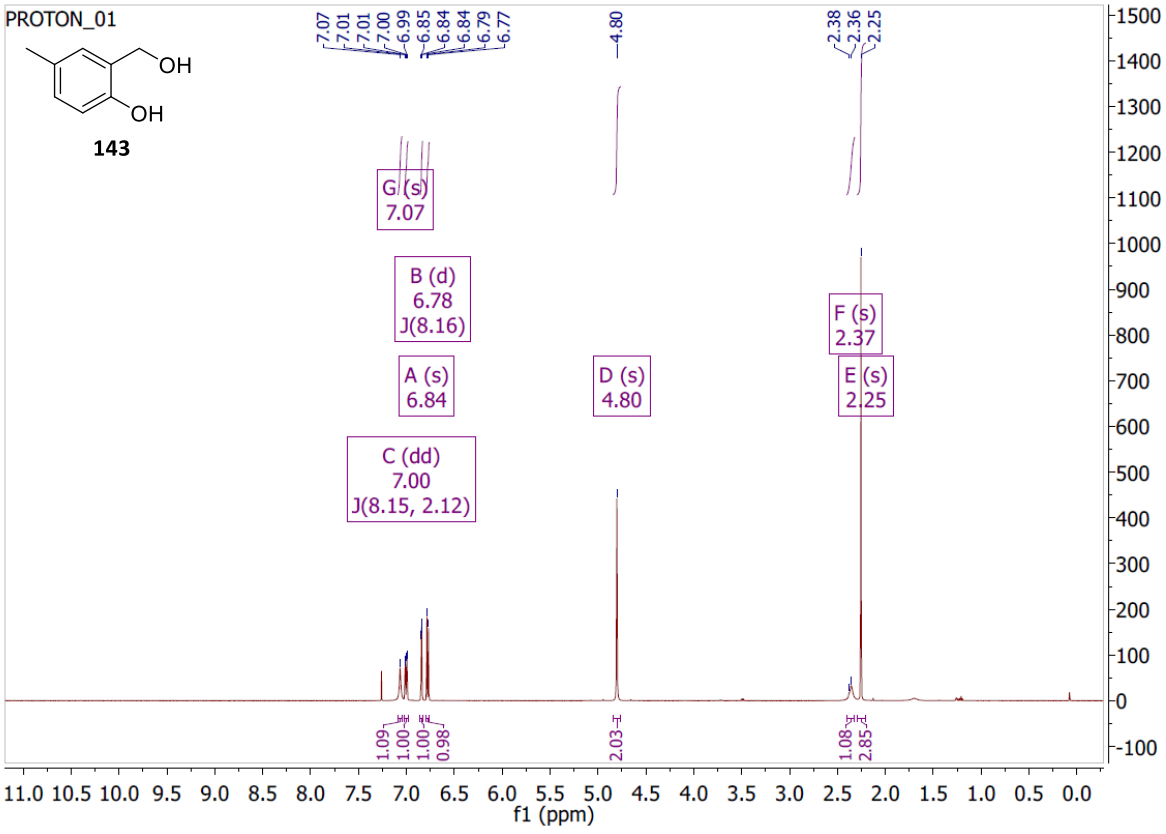
Generate Molecular Formula Parameters

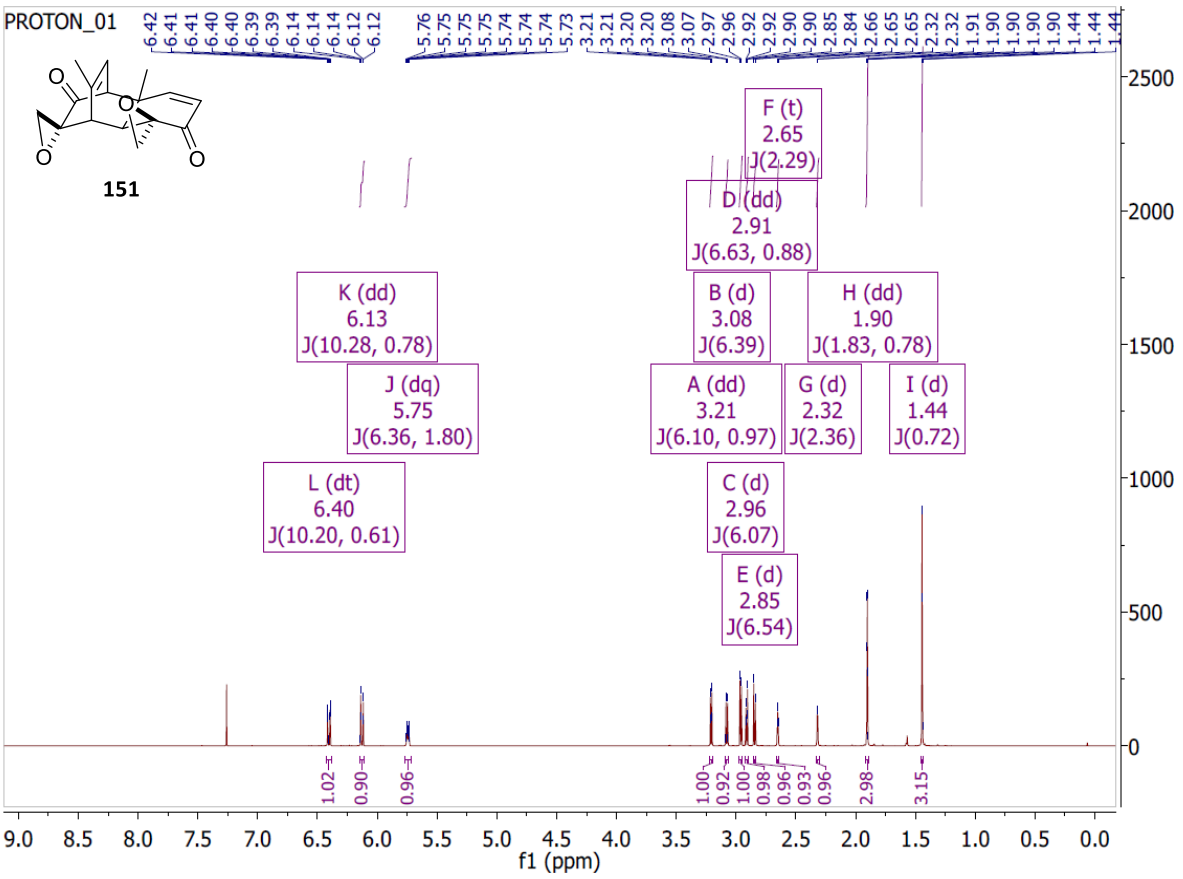
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

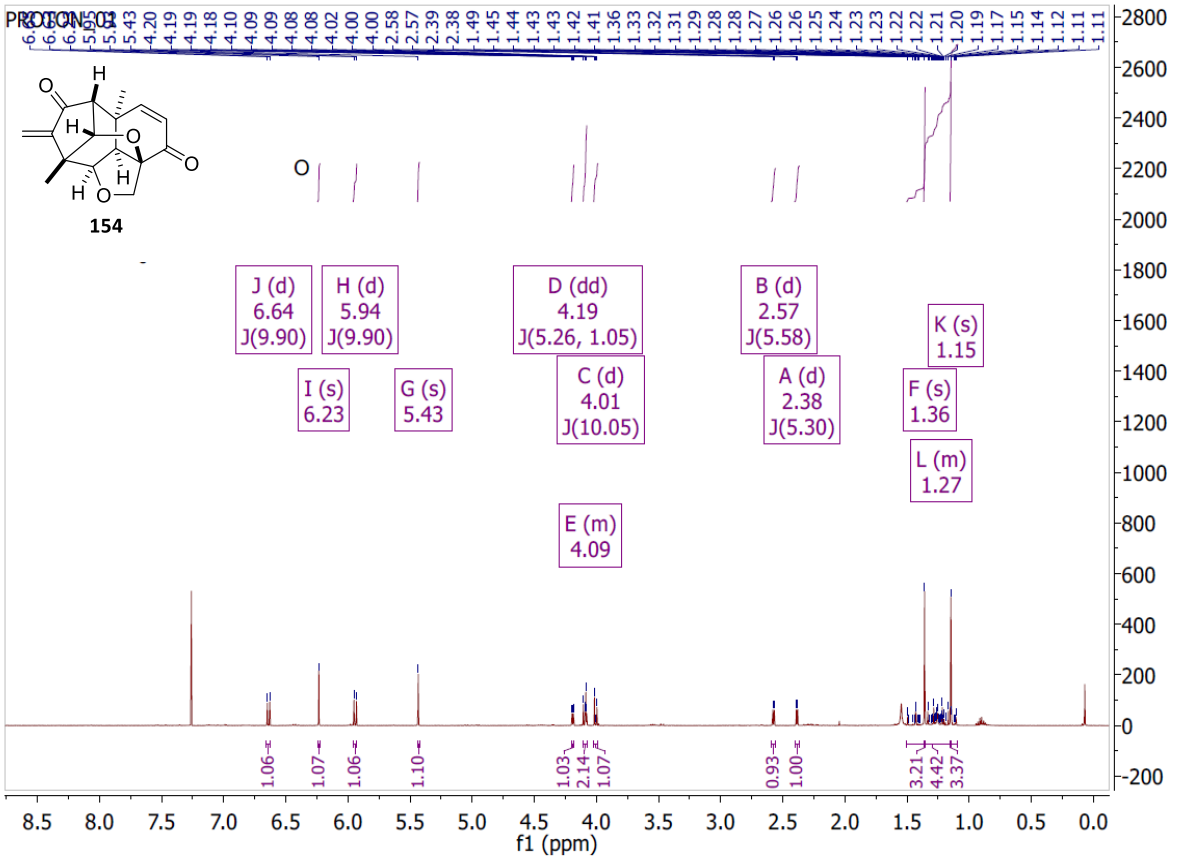
Expected Formula C14 H20 N2 O3 **Adduct(s):** H, Na

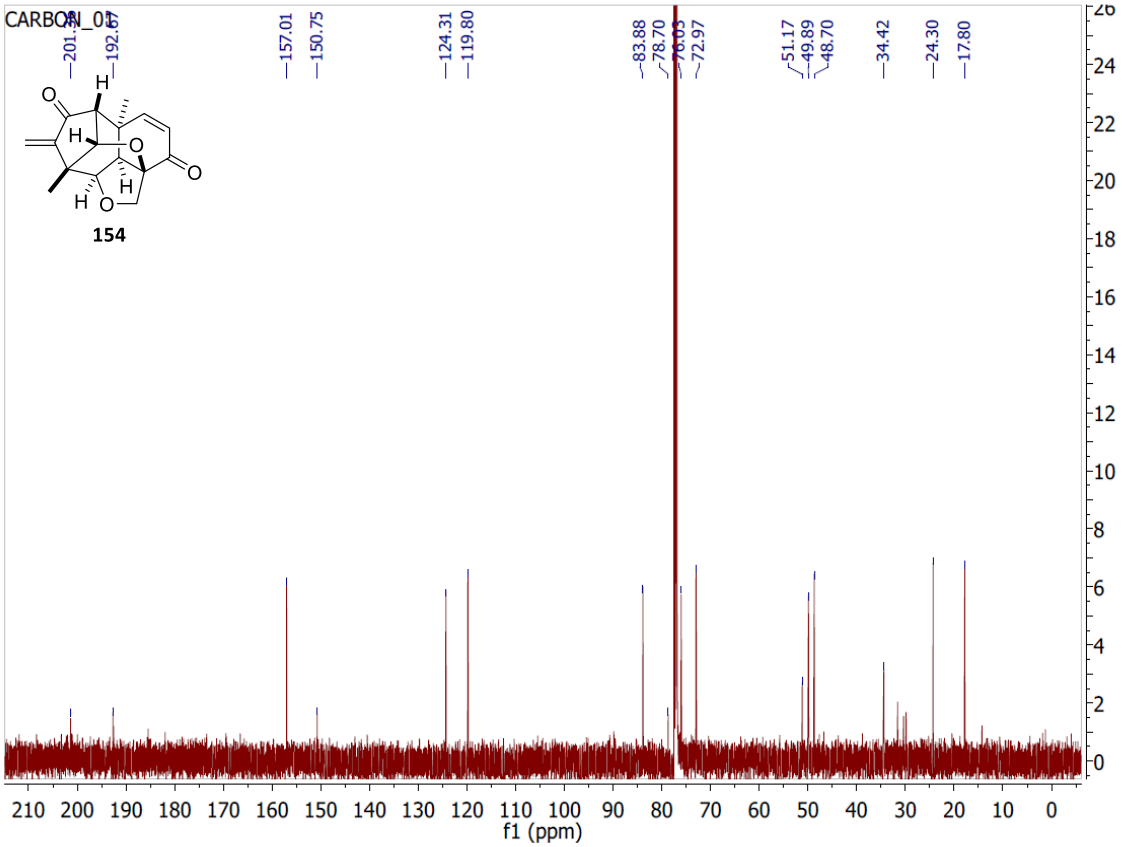
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula

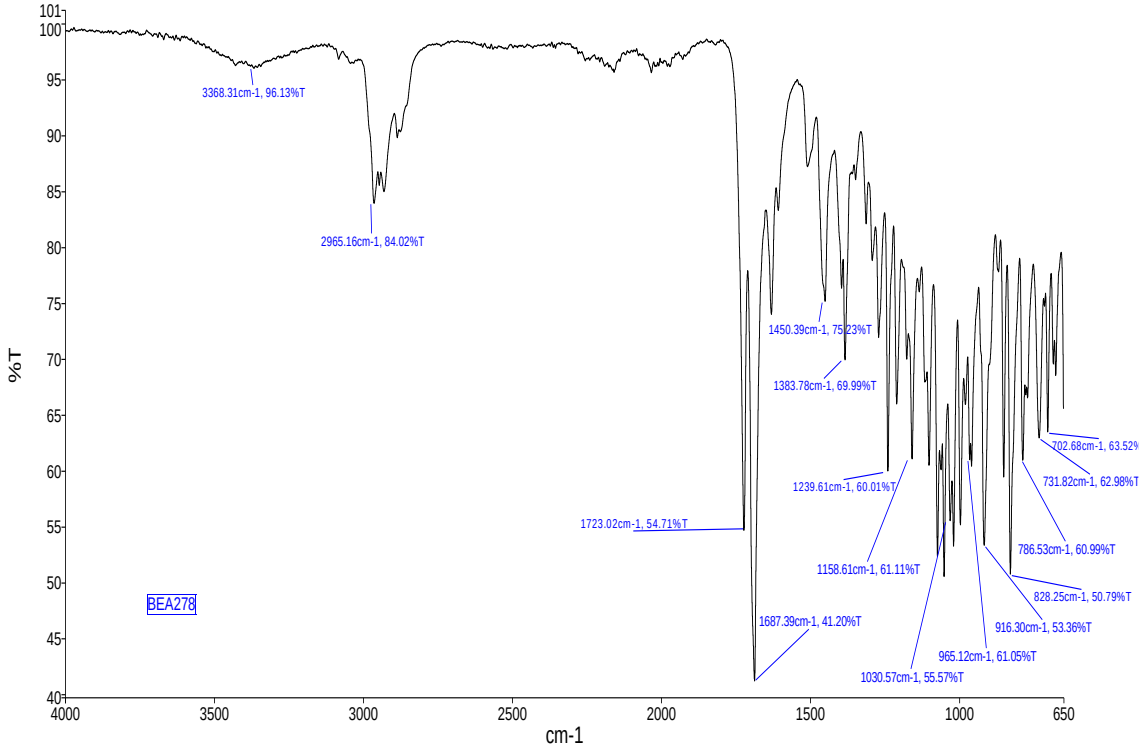
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication




PROTON_01
151
F (t)
2.65
J(2.29)
D (dd)
2.91
J(6.63, 0.88)
K (dd)
6.13
J(10.28, 0.78)
B (d)
3.08
J(6.39)
H (dd)
1.90
J(1.83, 0.78)
J (dq)
5.75
J(6.36, 1.80)
A (dd)
3.21
J(6.10, 0.97)
G (d)
2.32
J(2.36)
I (d)
1.44
J(0.72)
L (dt)
6.40
J(10.20, 0.61)
C (d)
2.96
J(6.07)
E (d)
2.85
J(6.54)
f1 (ppm)


154
J (d)
6.64
J(9.90)
H (d)
5.94
J(9.90)
D (dd)
4.19
J(5.26, 1.05)
B (d)
2.57
J(5.58)
K (s)
1.15
I (s)
6.23
G (s)
5.43
C (d)
4.01
J(10.05)
A (d)
2.38
J(5.30)
F (s)
1.36
L (m)
1.27
E (m)
4.09
f1 (ppm)

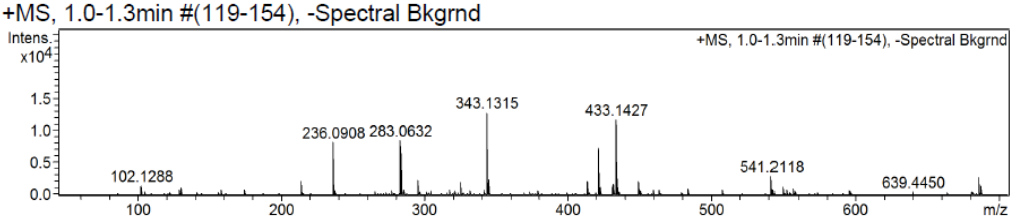

CARBON_01
201.21
192.67
157.01
150.75
124.31
119.80
83.88
78.70
76.03
72.97
51.17
49.89
48.70
34.42
24.30
17.80
154
f1 (ppm)


3368.31cm-1, 96.13%T
2965.16cm-1, 84.02%T
1723.02cm-1, 54.71%T
1687.39cm-1, 41.20%T
1450.39cm-1, 75.23%T
1383.78cm-1, 69.99%T
1239.61cm-1, 60.01%T
1158.61cm-1, 61.11%T
1030.57cm-1, 55.57%T
965.12cm-1, 61.05%T
916.30cm-1, 53.36%T
828.25cm-1, 50.79%T
786.53cm-1, 60.99%T
731.82cm-1, 62.98%T
702.68cm-1, 63.52%
BEA278
%T
cm-1

Confirmation of Expected Formula

Sample-ID	ba_sel_BEA278 B	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA278 B_356079_69_01_62082.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	28/02/2018 15:12:26
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	236.0908	8118	63.3	100	1749.7
2	283.0632	8438	65.8	375	712.3
3	295.0993	2243	17.5	79	175.1
4	343.1315	12829	100.0	755	1010.0
5	344.1348	2397	18.7	135	190.3
6	421.1483	7346	57.3	422	476.1
7	433.1427	11734	91.5	677	851.9
8	434.1470	2765	21.6	153	202.6
9	541.2118	2870	22.4	260	253.1
10	685.4417	2770	21.6	297	363.5

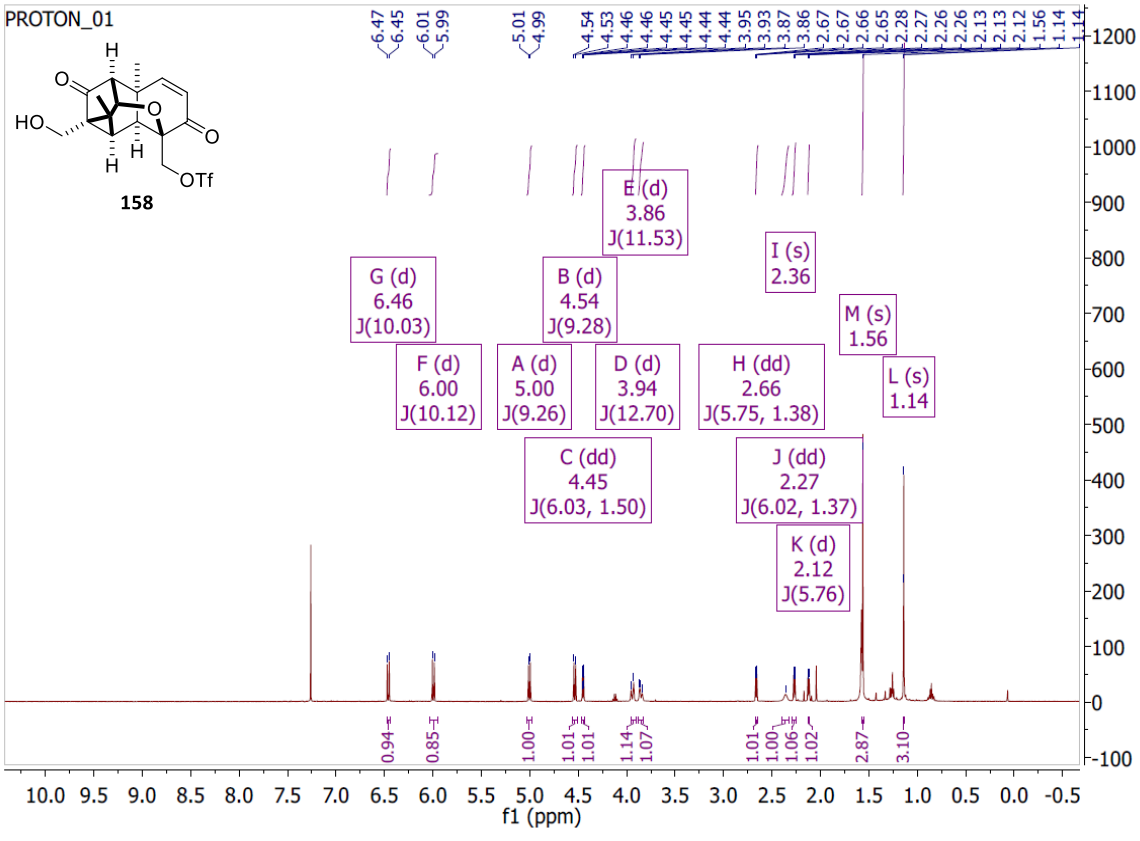
Generate Molecular Formula Parameters

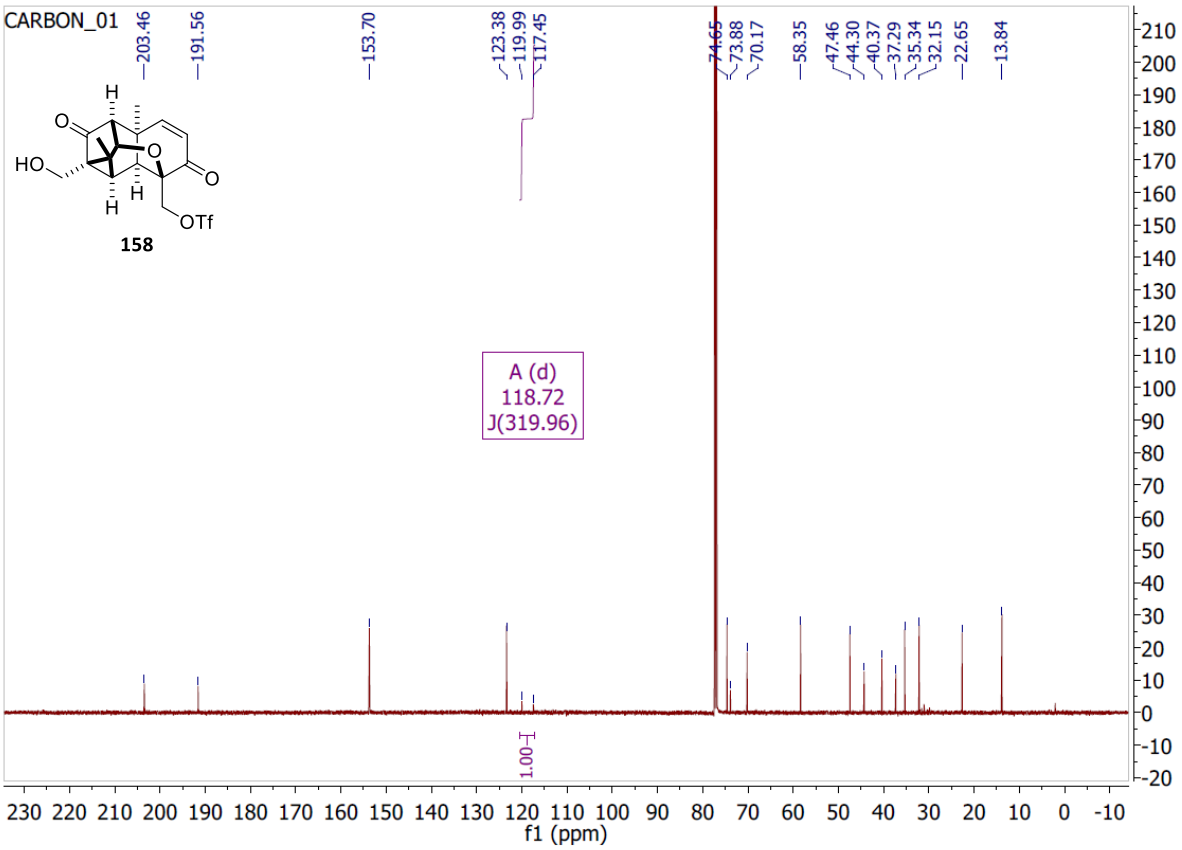
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

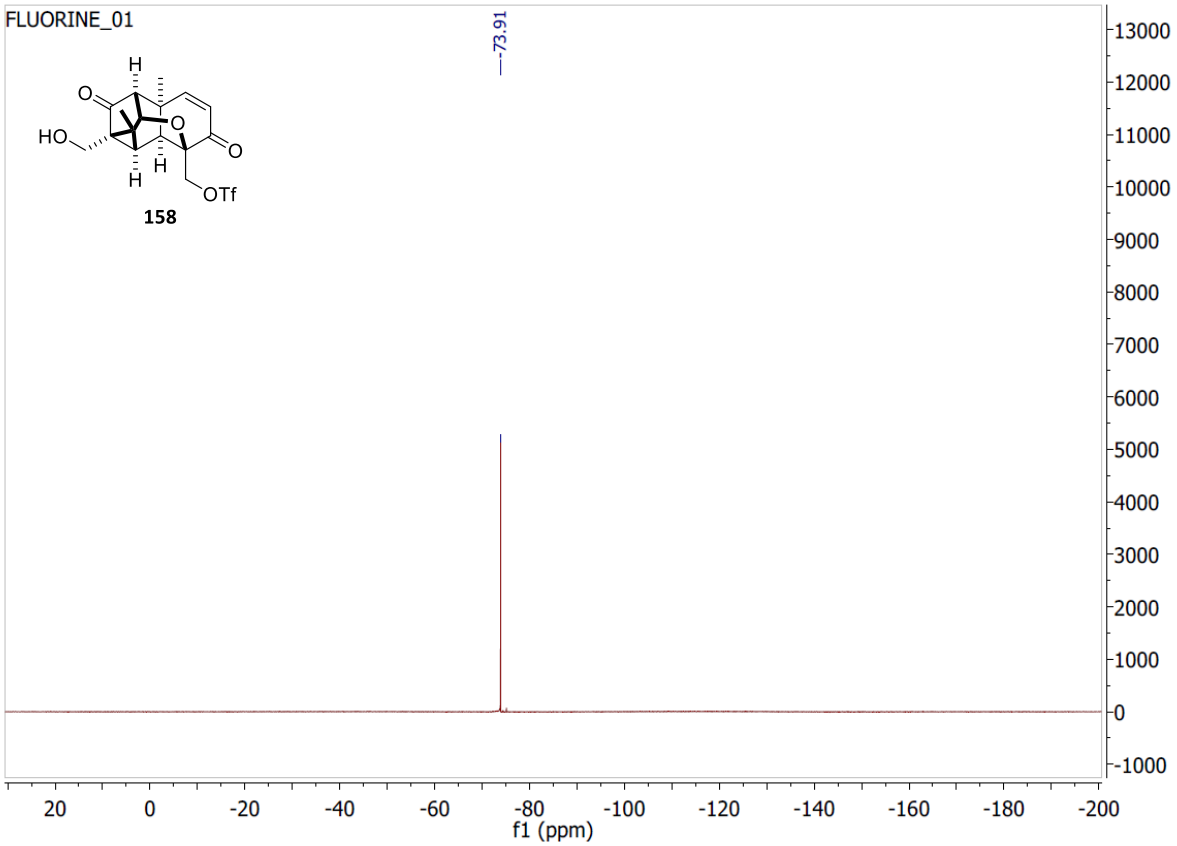
Expected Formula C16 H16 O4 **Adduct(s):** H, Na

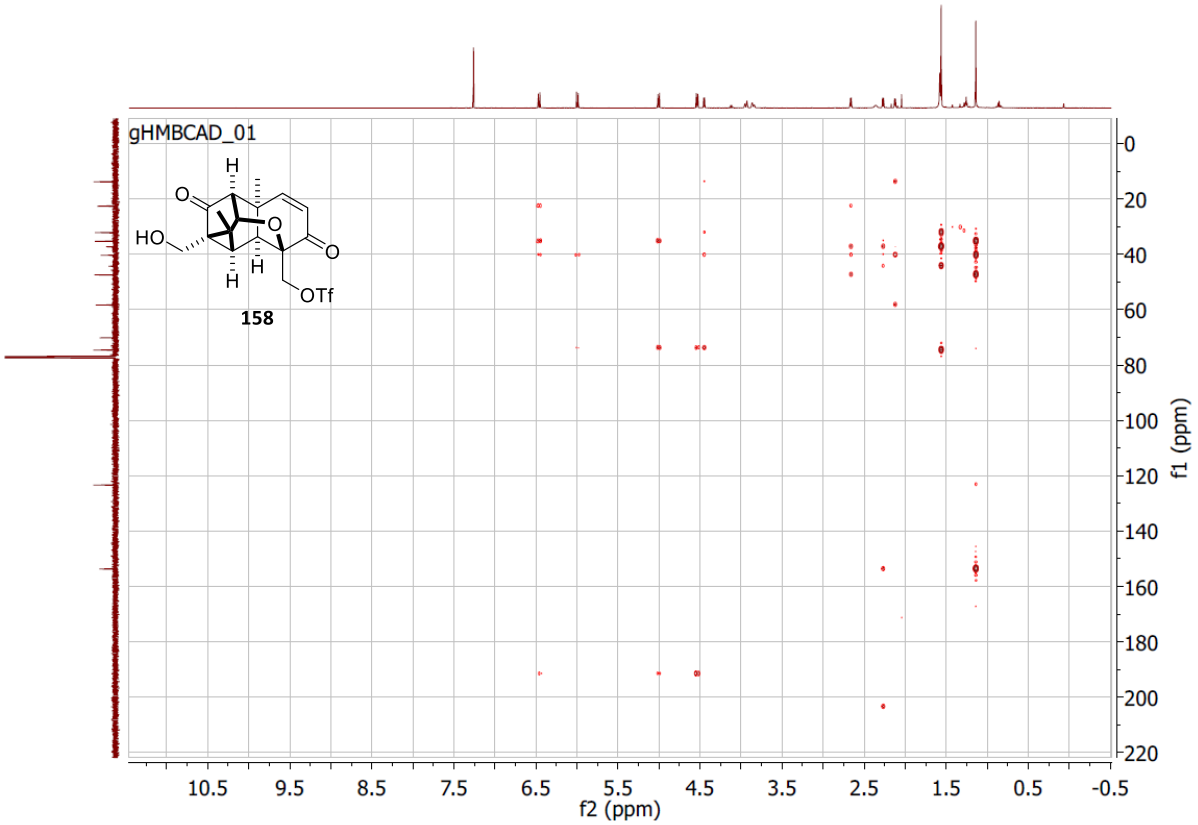
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	295.0993	295.0941	17.60	0.0244	C 16 H 16 Na 1 O 4

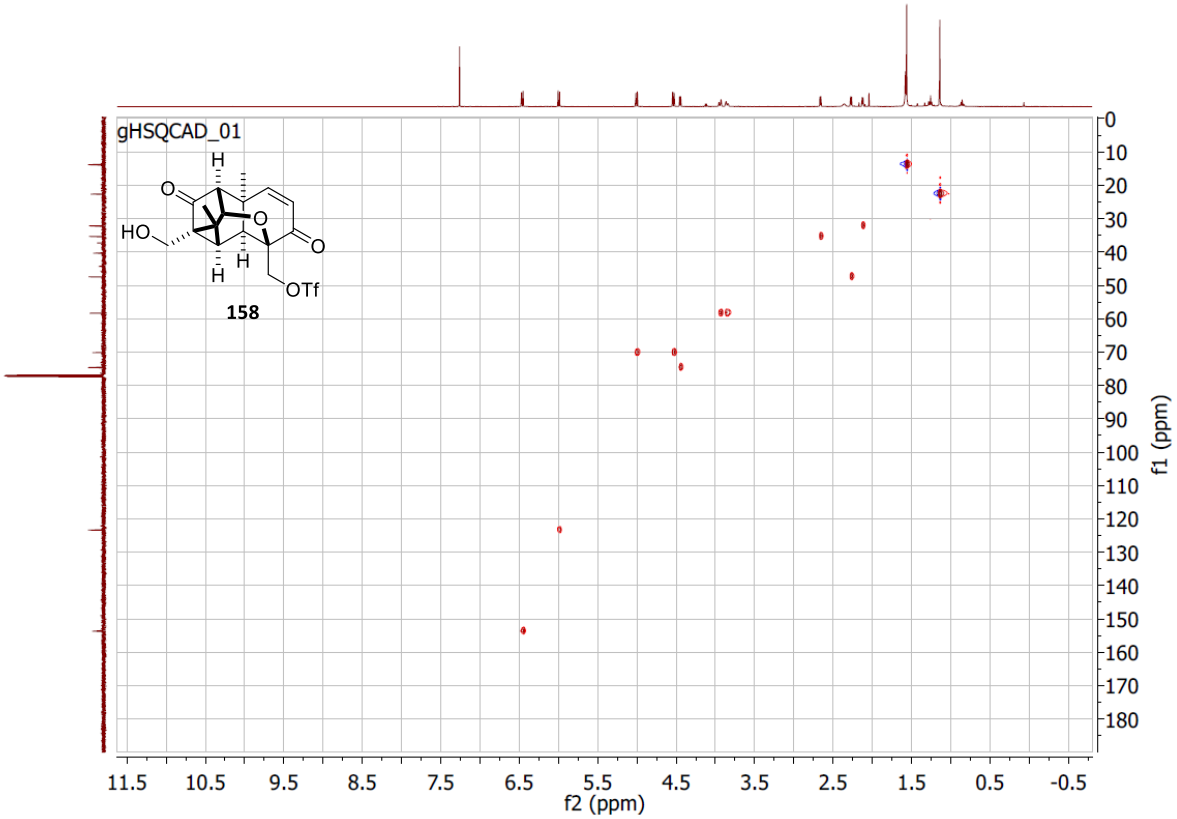
Note: Sigma fits < 0.05 indicates high probability of correct MF.

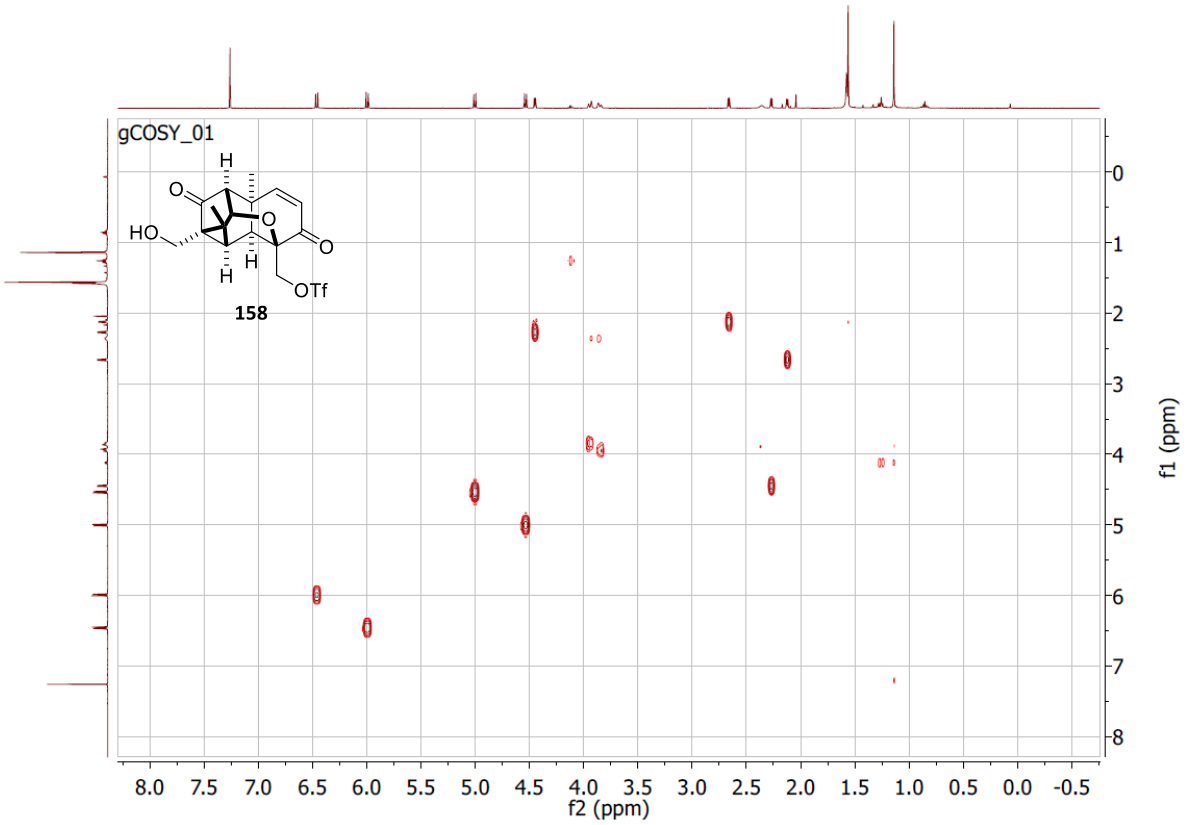


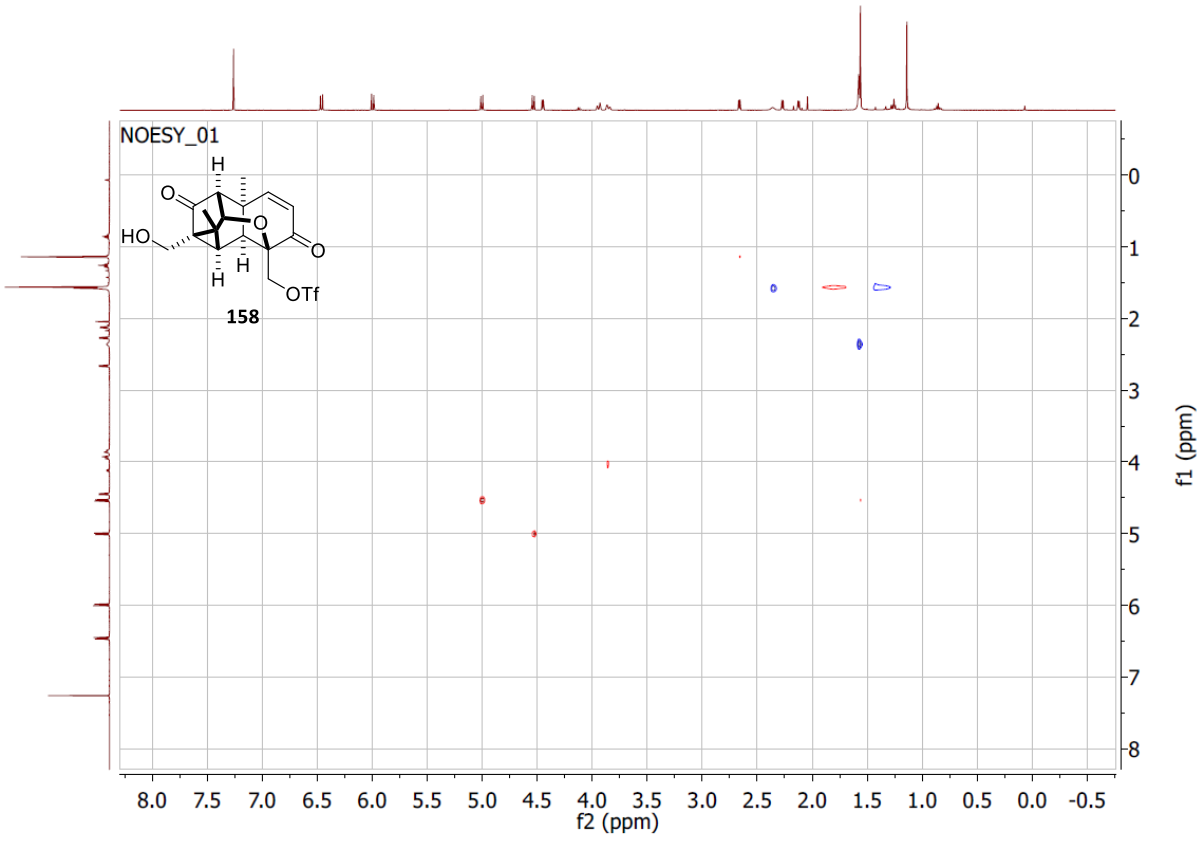

CARBON_01
203.46
191.56
153.70
123.38
119.99
117.45
74.65
73.88
70.17
58.35
47.46
44.30
40.37
37.29
35.34
32.15
22.65
13.84
158
A (d)
118.72
J(319.96)
1.00
f1 (ppm)

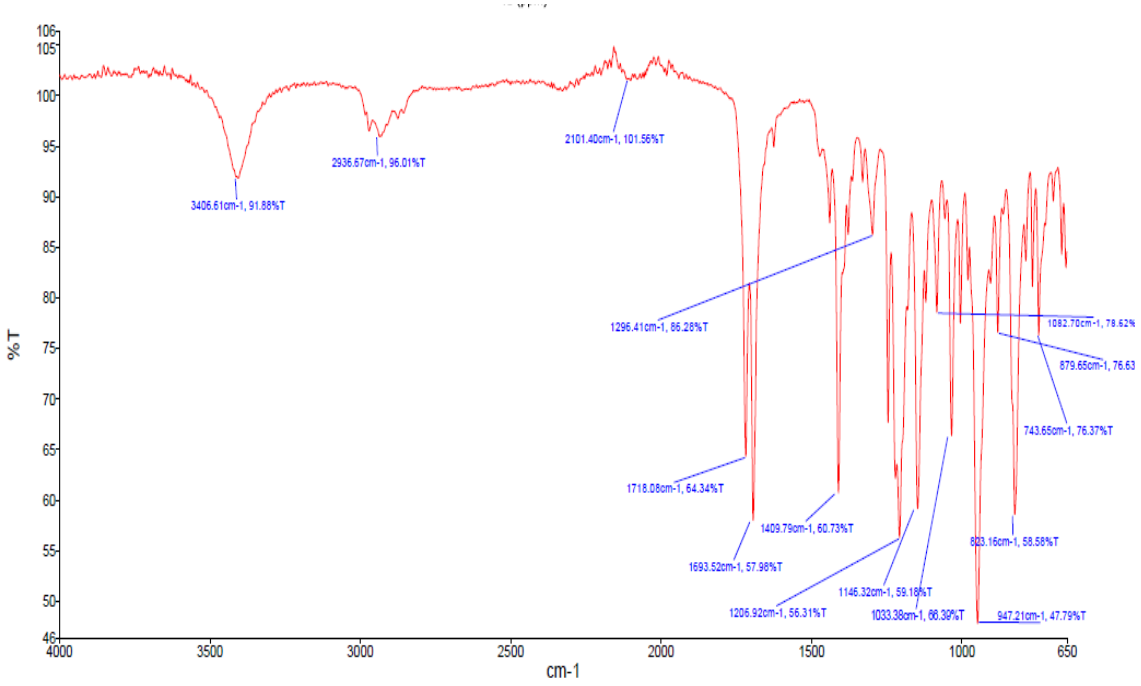

FLUORINE_01
-73.91
158
f1 (ppm)


gHMBCAD_01
158
f2 (ppm)
f1 (ppm)


gHSQCAD_01
158
f2 (ppm)
f1 (ppm)


gCOSY_01
158
f2 (ppm)
f1 (ppm)

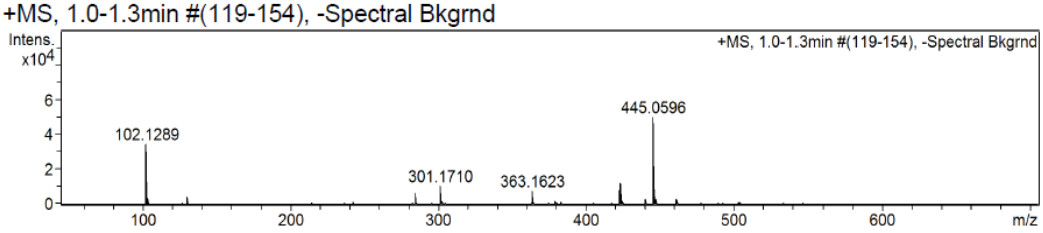

NOESY_01
158
f2 (ppm)
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_JLW024	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_JLW024_358362_43_01_64740.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	14/08/2018 11:25:38
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	102.1289	34438	69.4	514	21177.9
2	103.1319	3363	6.8	58	2021.6
3	130.1600	4191	8.4	82	2864.4
4	284.1242	6698	13.5	299	844.5
5	301.1710	10265	20.7	310	1470.7
6	363.1623	7463	15.0	400	851.4
7	422.2359	8282	16.7	534	540.5
8	423.0742	12056	24.3	818	781.6
9	445.0596	49609	100.0	3559	2738.7
10	446.0632	9080	18.3	608	497.9

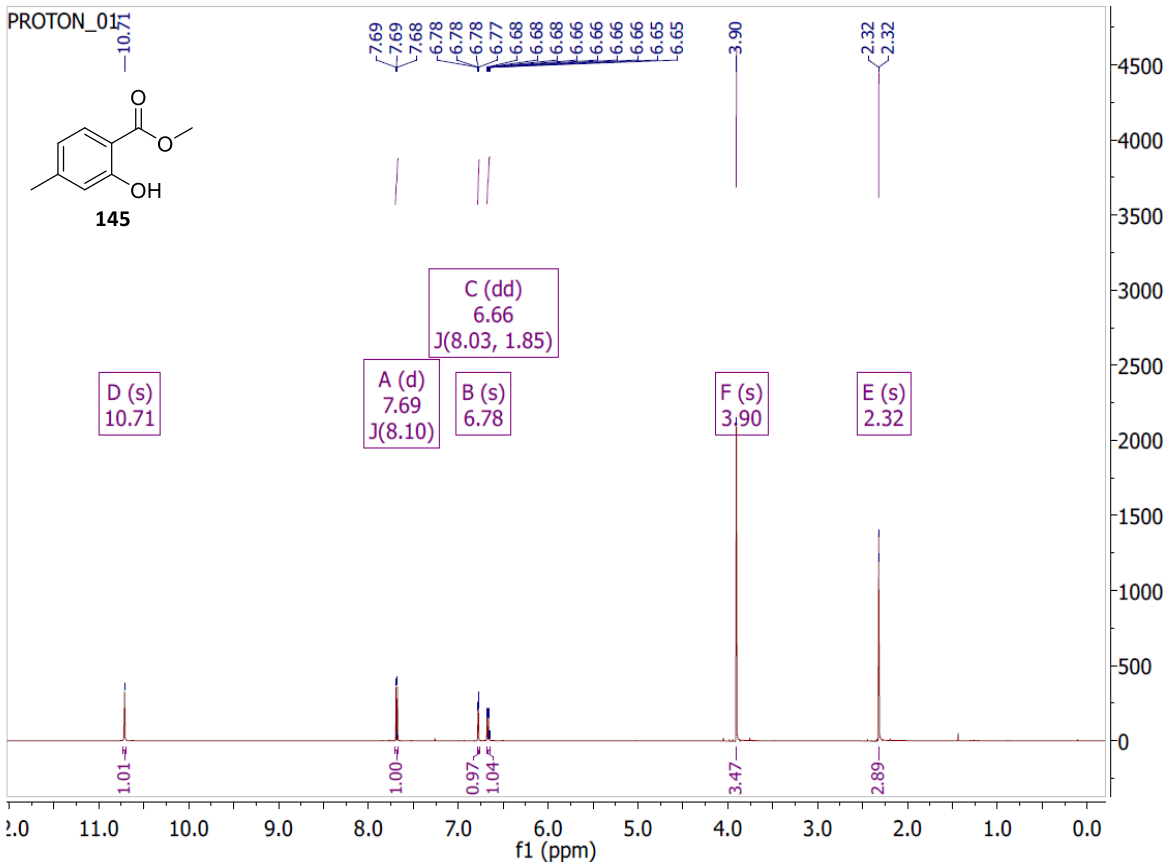
Generate Molecular Formula Parameters

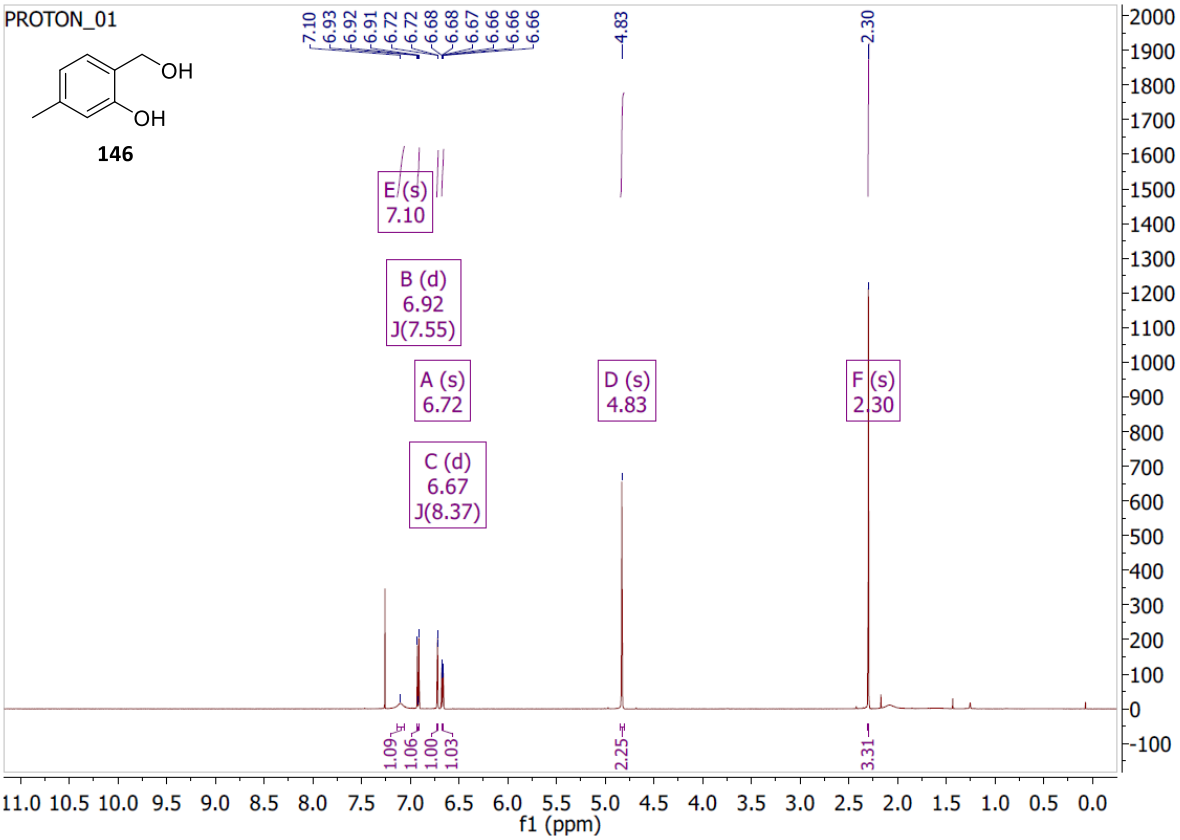
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

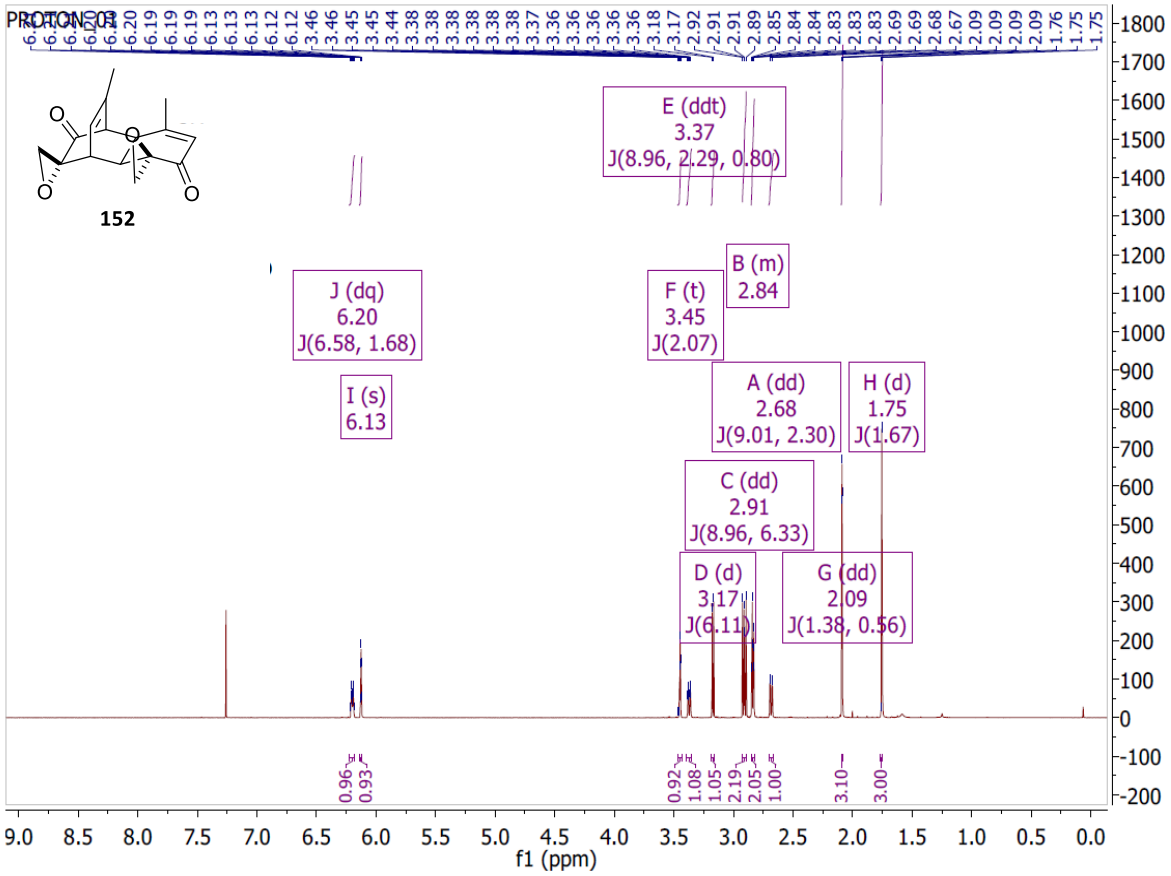
Expected Formula C17 H17 F3 O7 S1 **Adduct(s):** H, Na

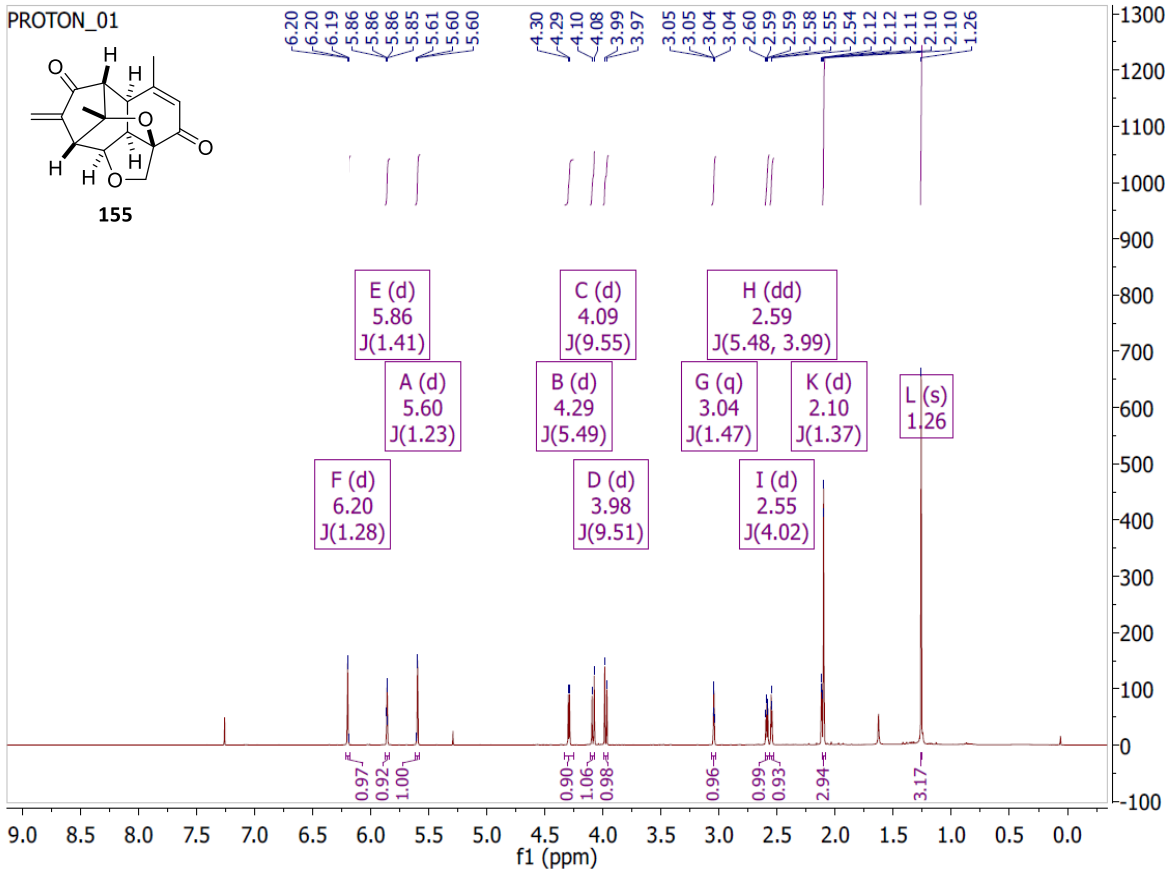
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	423.0742	423.0720	5.30	0.0140	C 17 H 18 F 3 O 7 S 1
1	445.0596	445.0539	12.90	0.0093	C 17 H 17 F 3 Na 1 O 7 S 1

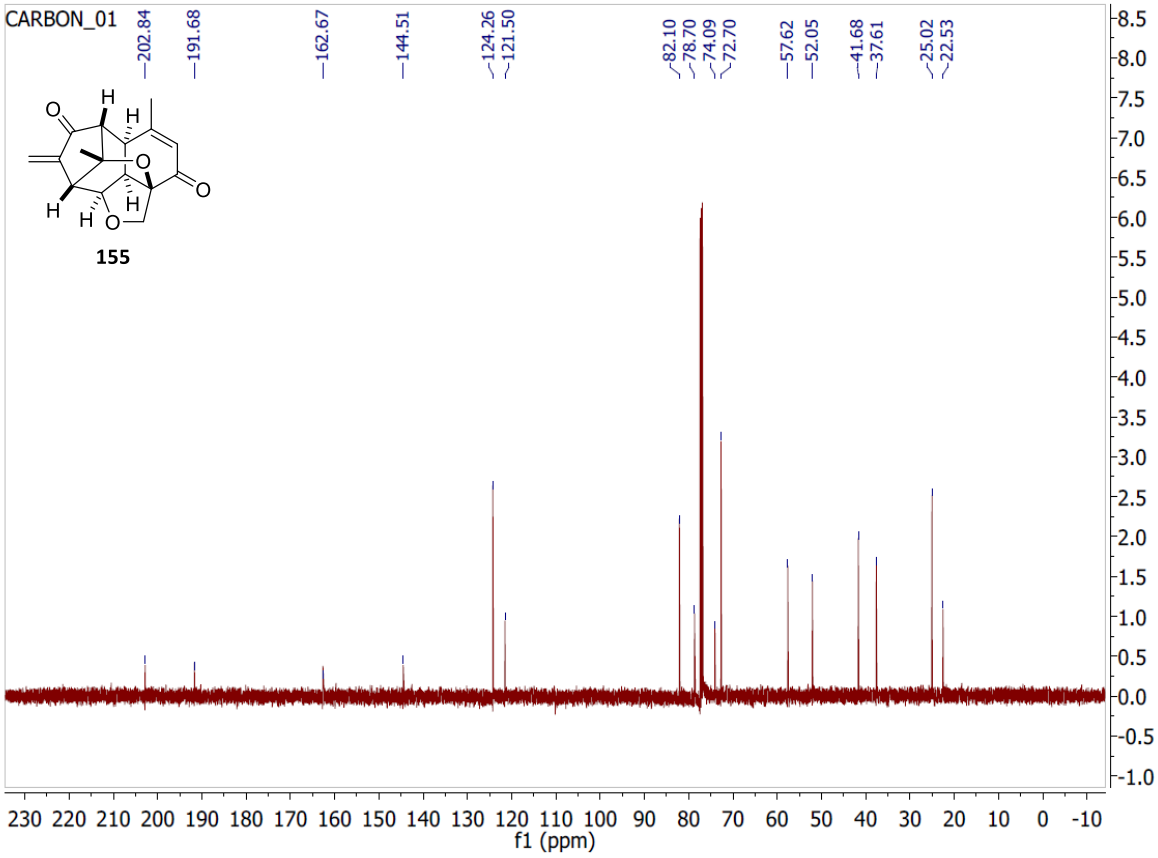
Note: Sigma fits < 0.05 indicates high probability of correct MF.

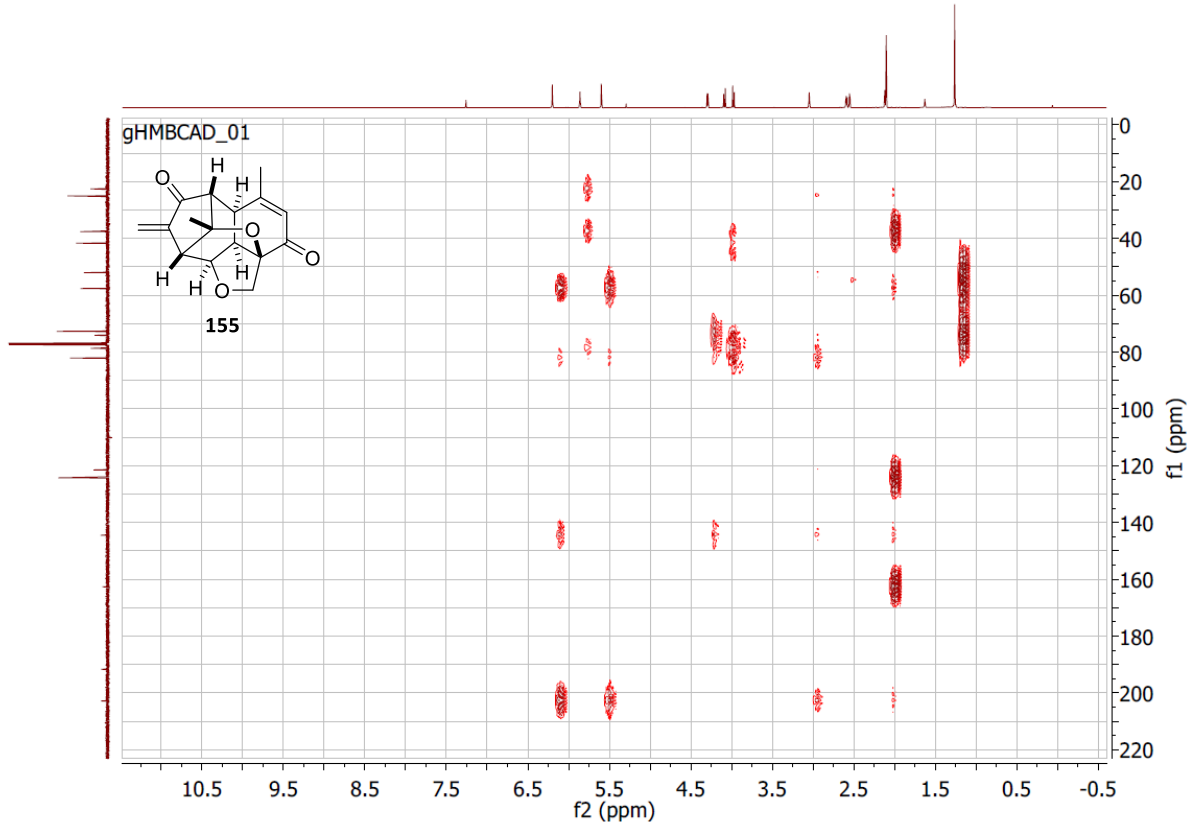

PROTON_01
10.71
7.69
7.69
7.68
6.78
6.78
6.78
6.77
6.68
6.68
6.68
6.66
6.66
6.66
6.66
6.65
6.65
3.90
2.32
2.32
O
O
OH
145
C (dd)
6.66
J(8.03, 1.85)
D (s)
10.71
A (d)
7.69
J(8.10)
B (s)
6.78
F (s)
3.90
E (s)
2.32
1.01
1.00
0.97
1.04
3.47
2.89
f1 (ppm)


PROTON_01
7.10
6.93
6.92
6.91
6.72
6.72
6.68
6.68
6.67
6.66
6.66
6.66
4.83
2.30
OH
OH
146
E (s)
7.10
B (d)
6.92
J(7.55)
A (s)
6.72
D (s)
4.83
F (s)
2.30
C (d)
6.67
J(8.37)
1.09
1.06
1.00
1.03
2.25
3.31
f1 (ppm)

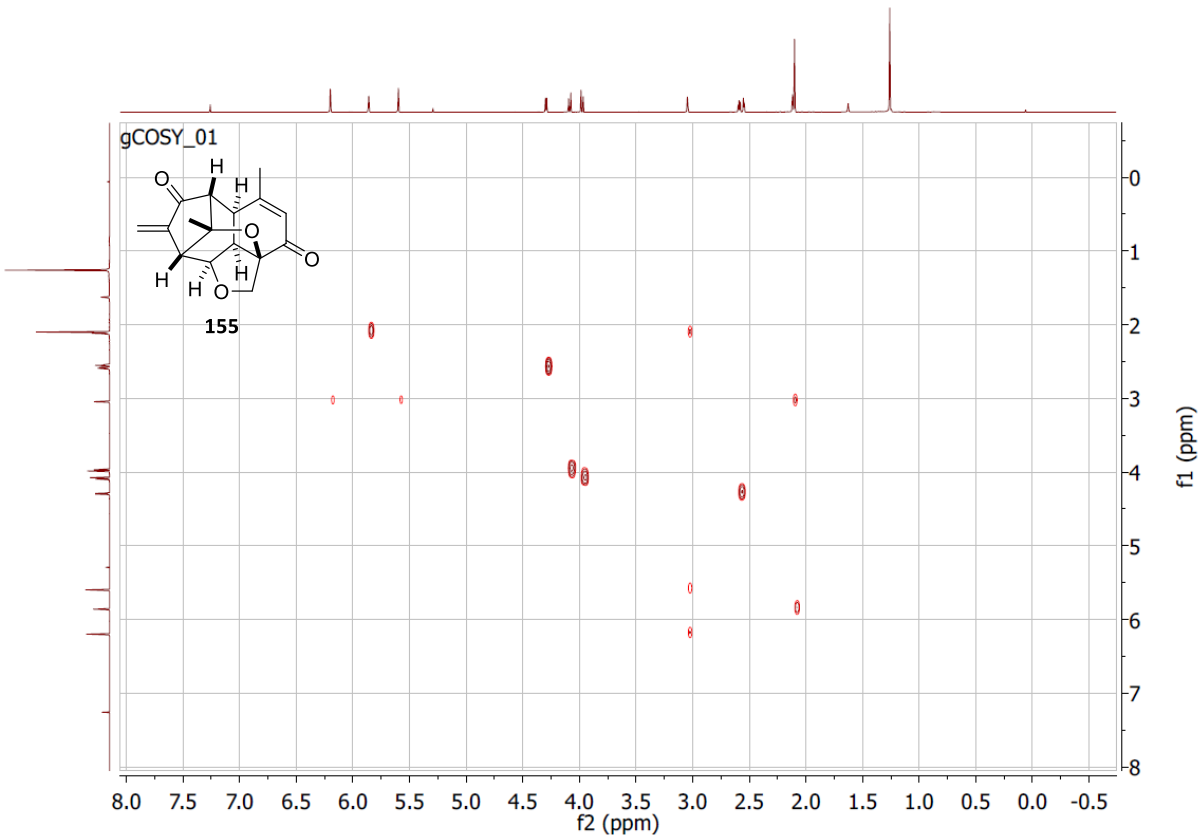

PROTON_03
152
E (ddt)
3.37
J(8.96, 2.29, 0.80)
B (m)
2.84
J (dq)
6.20
J(6.58, 1.68)
F (t)
3.45
J(2.07)
I (s)
6.13
A (dd)
2.68
J(9.01, 2.30)
H (d)
1.75
J(1.67)
C (dd)
2.91
J(8.96, 6.33)
D (d)
3.17
J(6.11)
G (dd)
2.09
J(1.38, 0.56)
f1 (ppm)

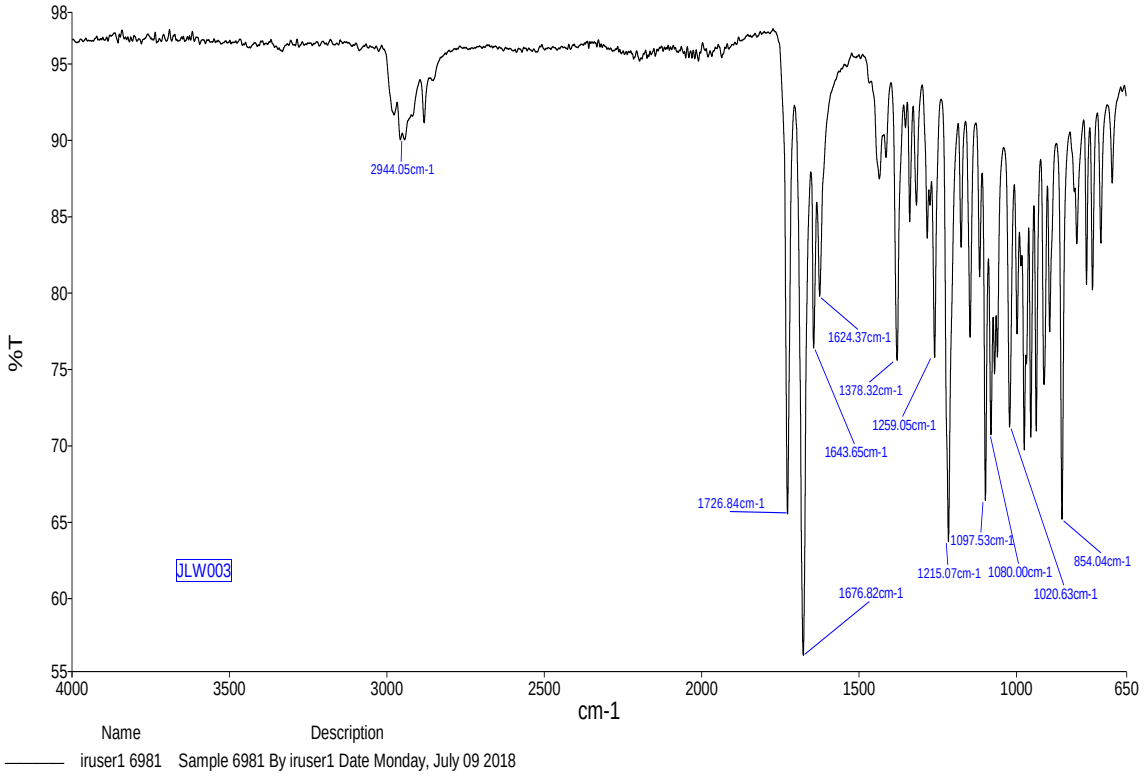

PROTON_01
155
E (d)
5.86
J(1.41)
C (d)
4.09
J(9.55)
H (dd)
2.59
J(5.48, 3.99)
A (d)
5.60
J(1.23)
B (d)
4.29
J(5.49)
G (q)
3.04
J(1.47)
K (d)
2.10
J(1.37)
L (s)
1.26
F (d)
6.20
J(1.28)
D (d)
3.98
J(9.51)
I (d)
2.55
J(4.02)
f1 (ppm)


CARBON_01
202.84
191.68
162.67
144.51
124.26
121.50
82.10
78.70
74.09
72.70
57.62
52.05
41.68
37.61
25.02
22.53
155
f1 (ppm)


gHMBCAD_01
155
f2 (ppm)
f1 (ppm)


gHSQCAD_01
155
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f2 (ppm)
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180
f1 (ppm)

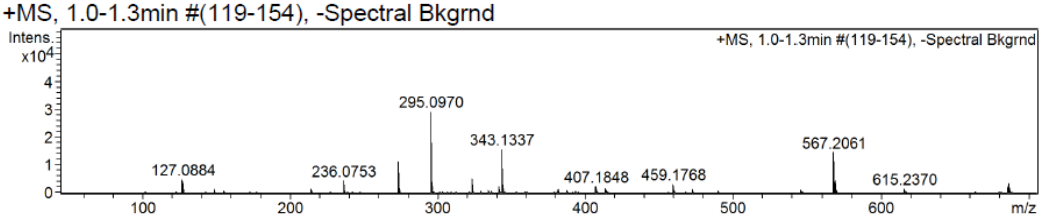

gCOSY_01
155
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f2 (ppm)
0 1 2 3 4 5 6 7 8
f1 (ppm)



Confirmation of Expected Formula

Sample-ID	ba_sel_JLW003	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_JLW003_358359_40_01_64737.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	14/08/2018 11:15:02
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	127.0884	4879	16.7	122	4199.6
2	236.0753	4504	15.4	113	1164.7
3	273.1154	11407	39.0	441	1222.4
4	295.0970	29255	100.0	846	2403.2
5	296.0999	4066	13.9	137	332.6
6	323.1257	5136	17.6	264	376.8
7	343.1337	15669	53.6	852	1199.4
8	567.2061	14556	49.8	1281	1979.8
9	568.2075	4613	15.8	432	633.8
10	685.4379	3569	12.2	467	466.7

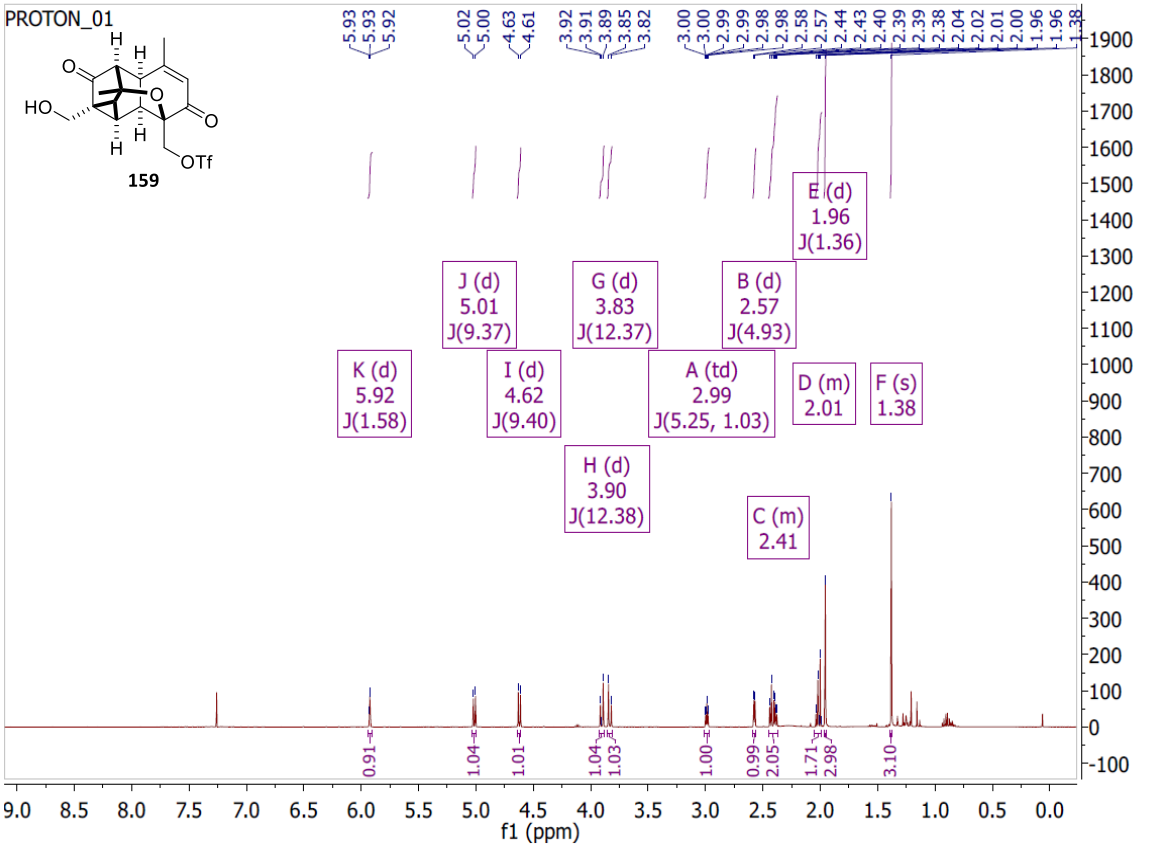
Generate Molecular Formula Parameters

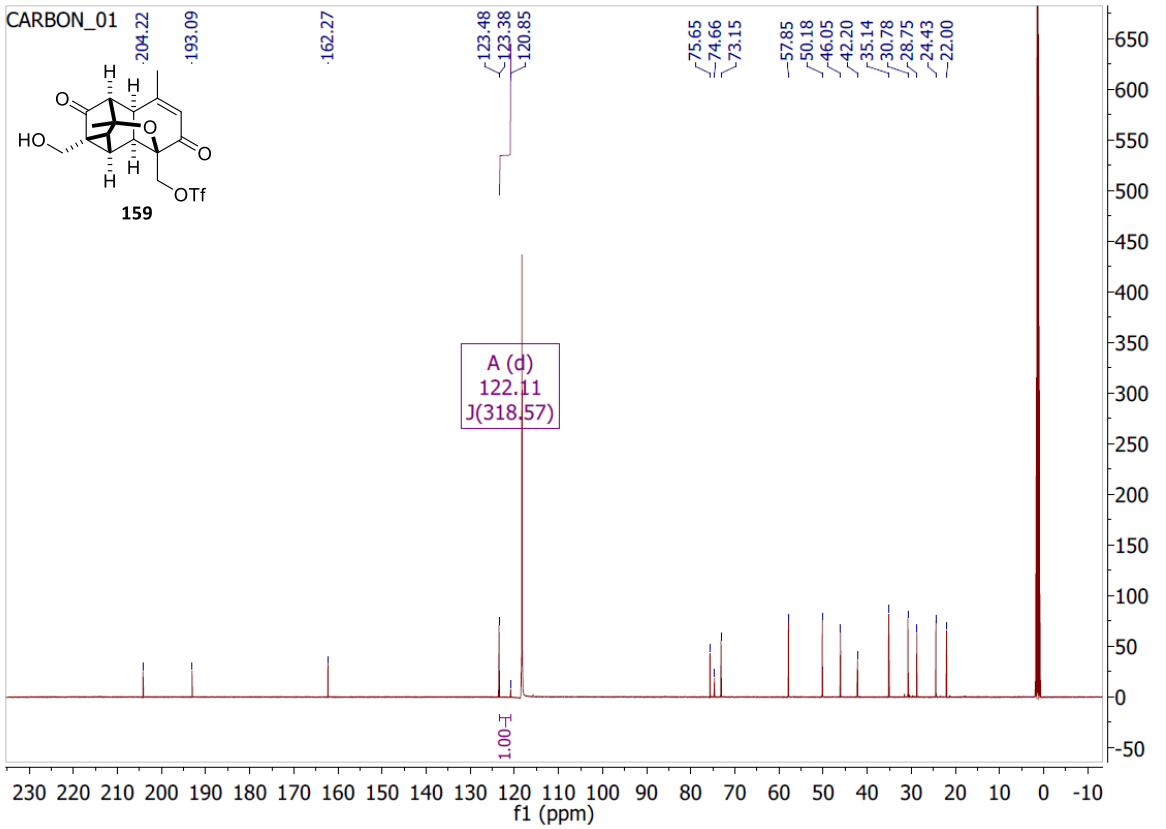
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

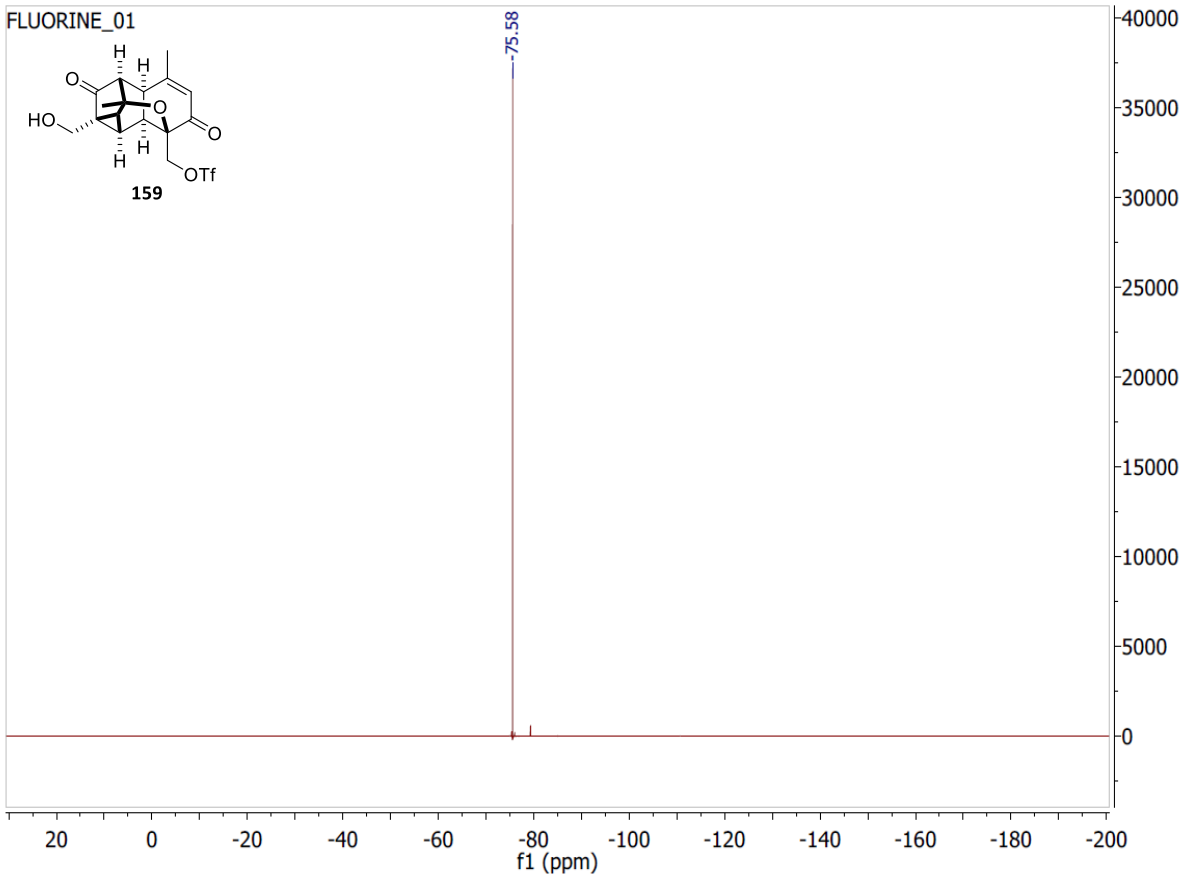
Expected Formula C16 H16 O4 **Adduct(s):** H, Na

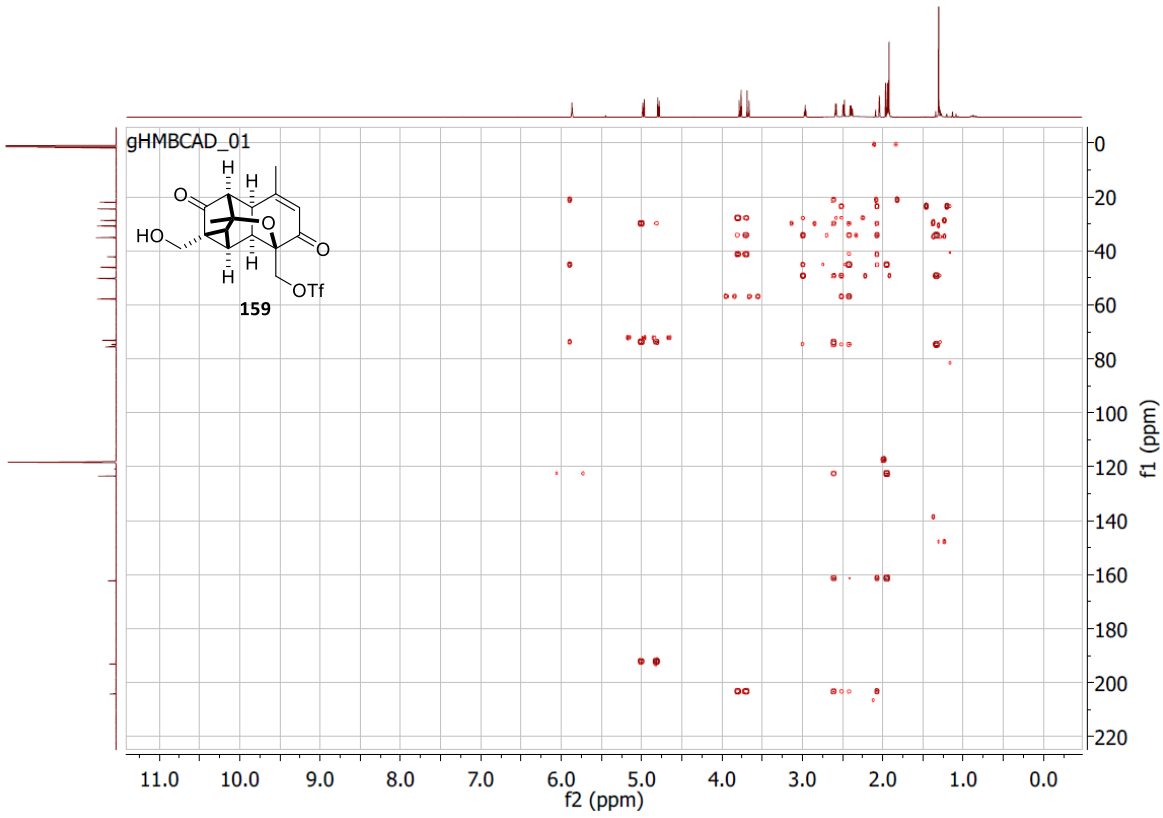
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	273.1154	273.1121	11.90	0.0079	C 16 H 17 O 4
1	295.0970	295.0941	9.80	0.0200	C 16 H 16 Na 1 O 4

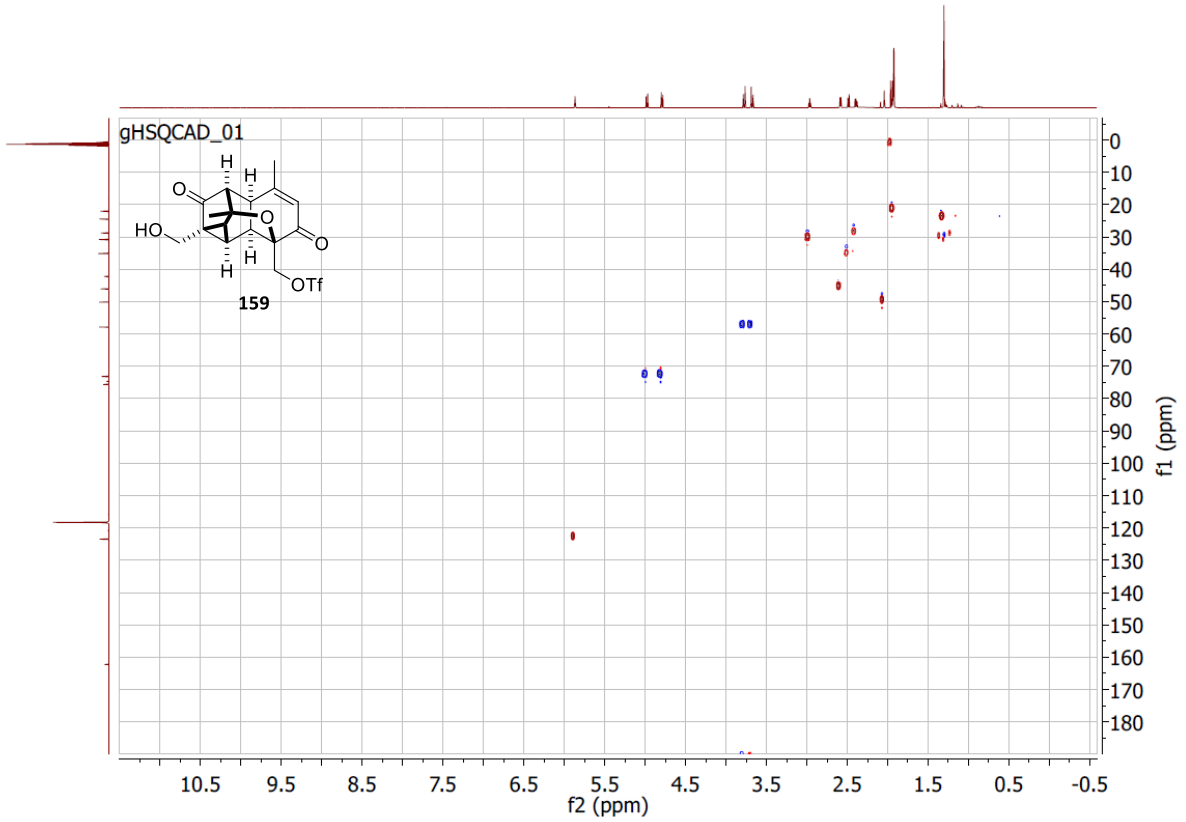
Note: Sigma fits < 0.05 indicates high probability of correct MF.

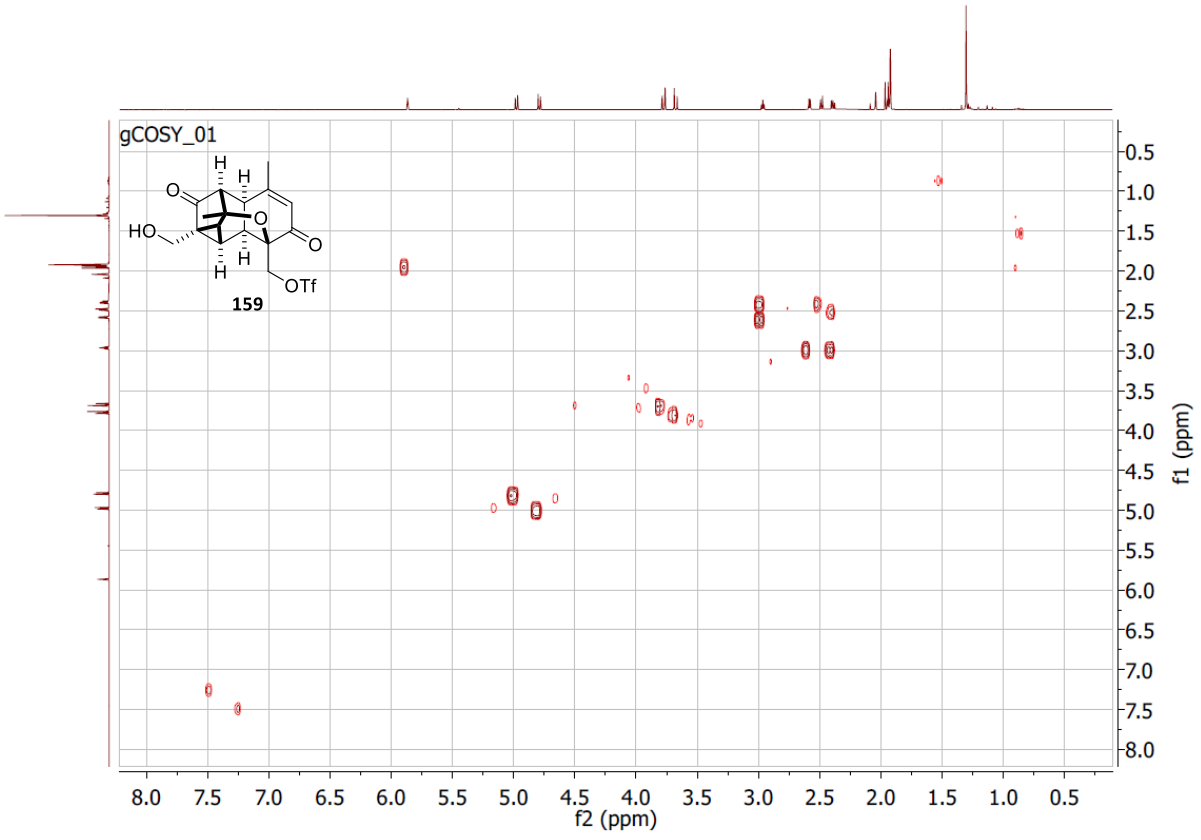

PROTON_01
159
E (d)
1.96
J(1.36)
J (d)
5.01
J(9.37)
G (d)
3.83
J(12.37)
B (d)
2.57
J(4.93)
K (d)
5.92
J(1.58)
I (d)
4.62
J(9.40)
A (td)
2.99
J(5.25, 1.03)
D (m)
2.01
F (s)
1.38
H (d)
3.90
J(12.38)
C (m)
2.41
f1 (ppm)

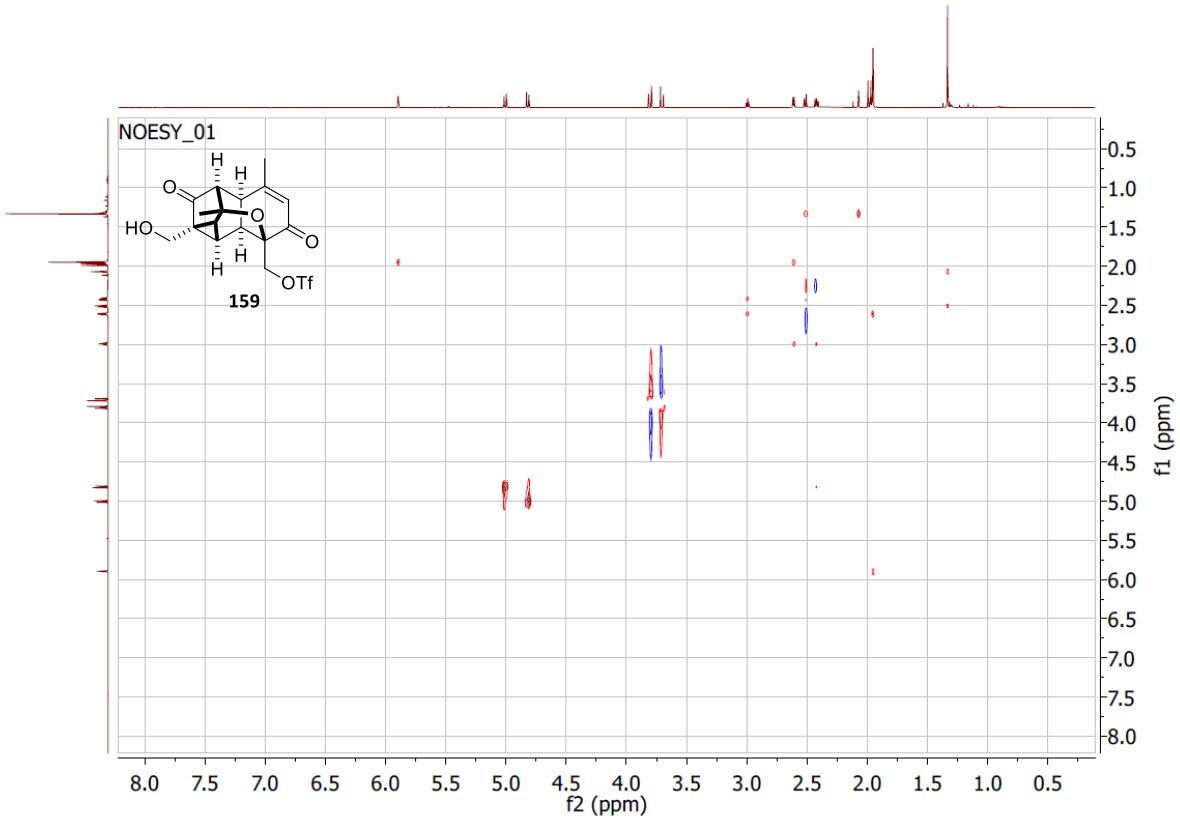

CARBON_01
159
A (d)
122.11
J(318.57)
f1 (ppm)

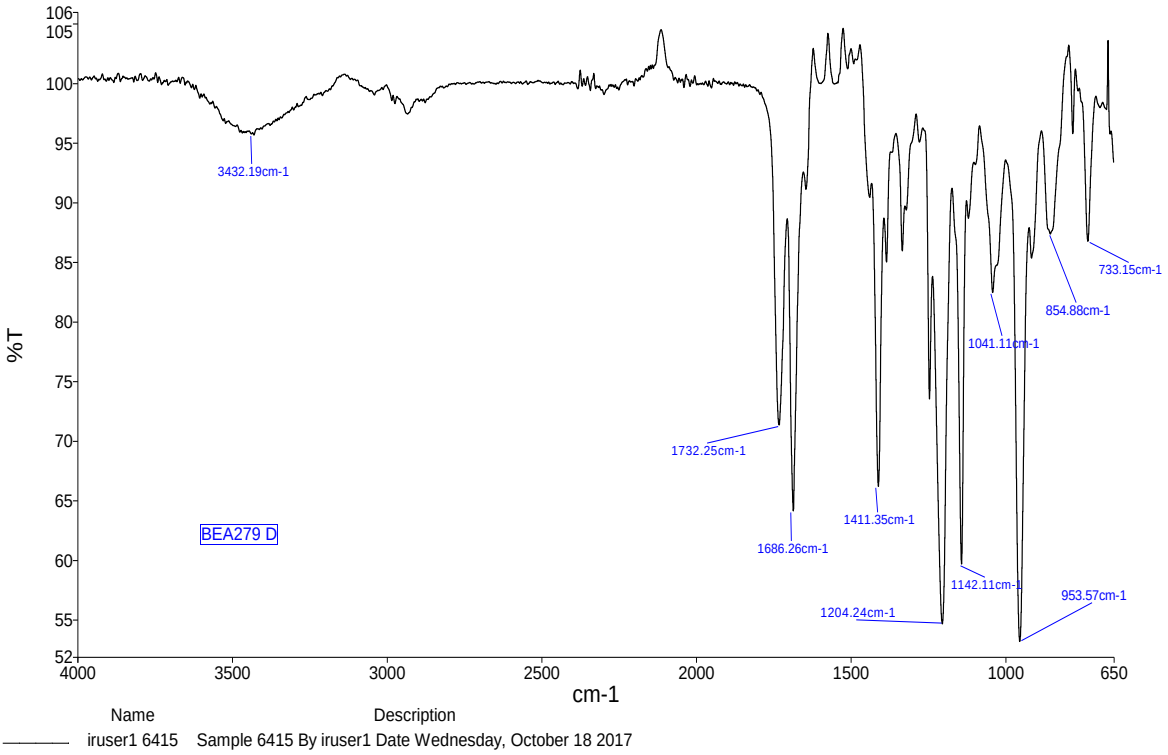

FLUORINE_01
-75.58
159
40000
35000
30000
25000
20000
15000
10000
5000
0
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)


gHMBCAD_01
159
0
20
40
60
80
100
120
140
160
180
200
220
f1 (ppm)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f2 (ppm)


gHSQCAD_01
HO
OTf
159
f2 (ppm)
f1 (ppm)


gCOSY_01
HO
OTf
159
f2 (ppm)
f1 (ppm)

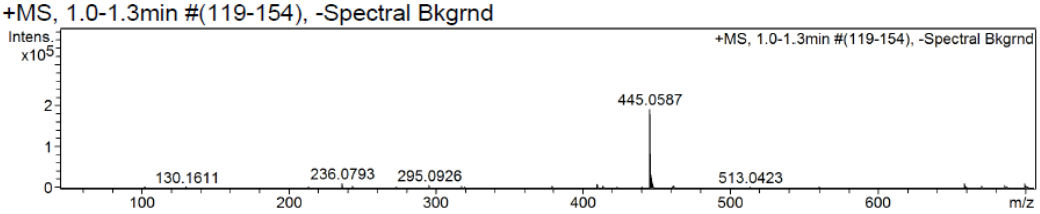

NOESY_01
HO
O
O
O
H
H
H
H
OTf
159
f2 (ppm)
f1 (ppm)


%T
cm-1
3432.19cm-1
1732.25cm-1
1686.26cm-1
1411.35cm-1
1204.24cm-1
1142.11cm-1
1041.11cm-1
953.57cm-1
854.88cm-1
733.15cm-1
BEA279 D
Name
Description
iruser1 6415
Sample 6415 By iruser1 Date Wednesday, October 18 2017

Confirmation of Expected Formula

Sample-ID	ba_sel_BEA279 D	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_BEA279 D_353872_42_01_59559.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	19/10/2017 14:34:25
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	236.0793	12514	6.5	248	1098.1
2	295.0926	7814	4.1	355	552.9
3	379.1170	5209	2.7	331	363.2
4	409.1958	9012	4.7	189	544.1
5	445.0587	192624	100.0	14524	5752.6
6	446.0591	34211	17.8	2616	1002.9
7	447.0555	13031	6.8	978	375.1
8	658.1401	11177	5.8	1334	604.5
9	685.4378	7395	3.8	984	308.4
10	699.1497	11966	6.2	1663	499.4

Generate Molecular Formula Parameters

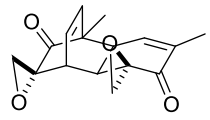
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C17 H17 F3 O7 S1 **Adduct(s):** H, Na

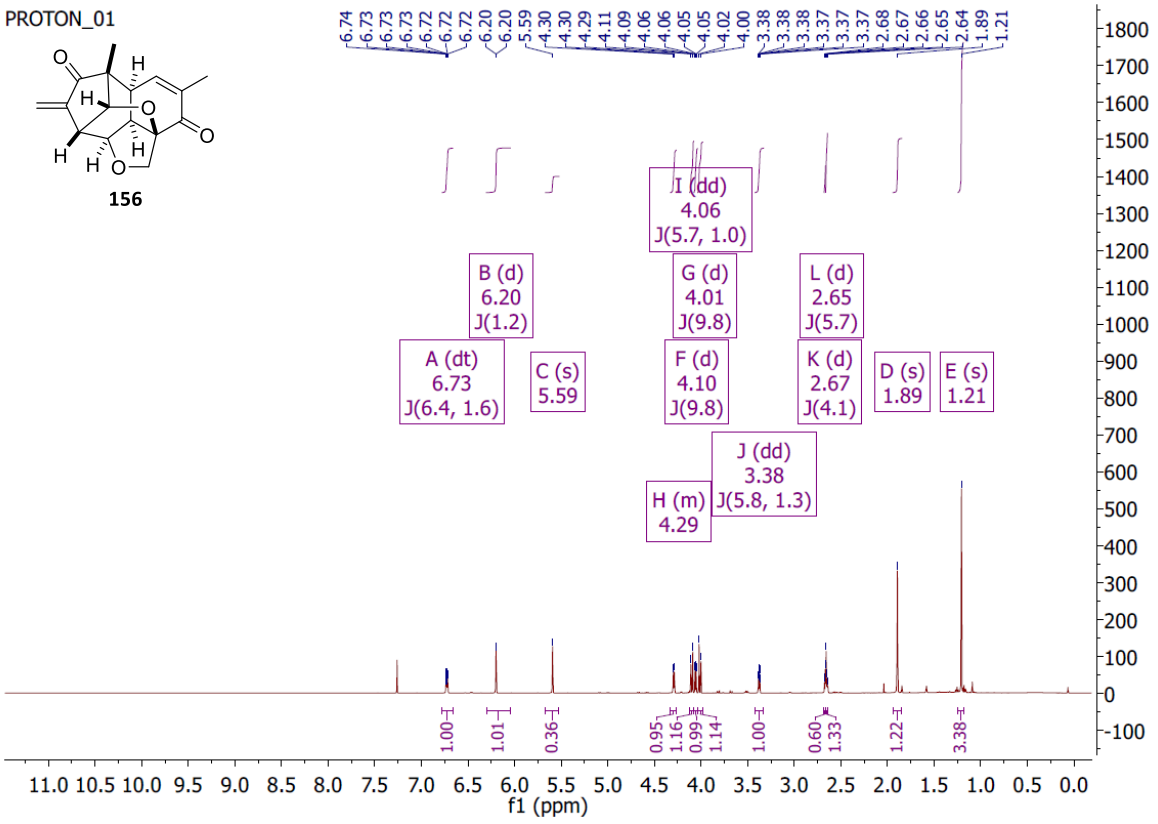
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	423.0719	423.0720	-0.20	0.0471	C 17 H 18 F 3 O 7 S 1
1	445.0587	445.0539	10.60	0.0086	C 17 H 17 F 3 Na 1 O 7 S 1

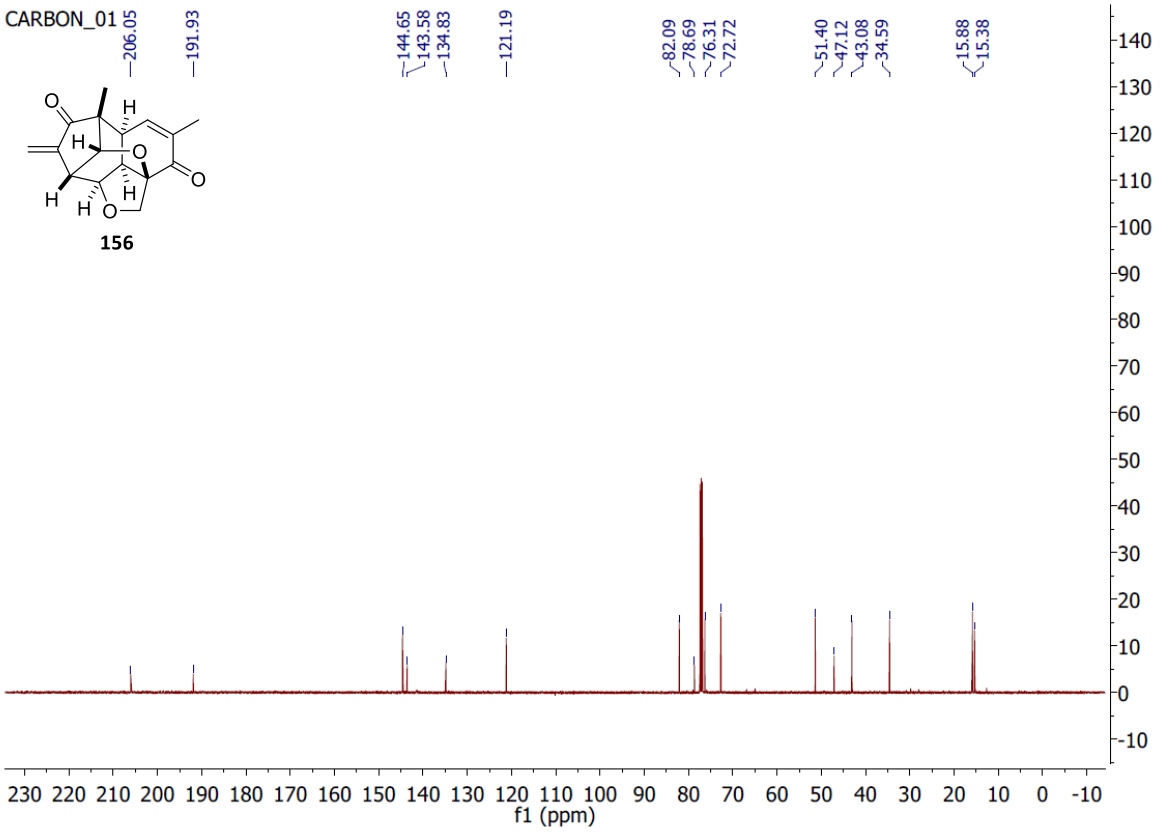
Note: Sigma fits < 0.05 indicates high probability of correct MF.

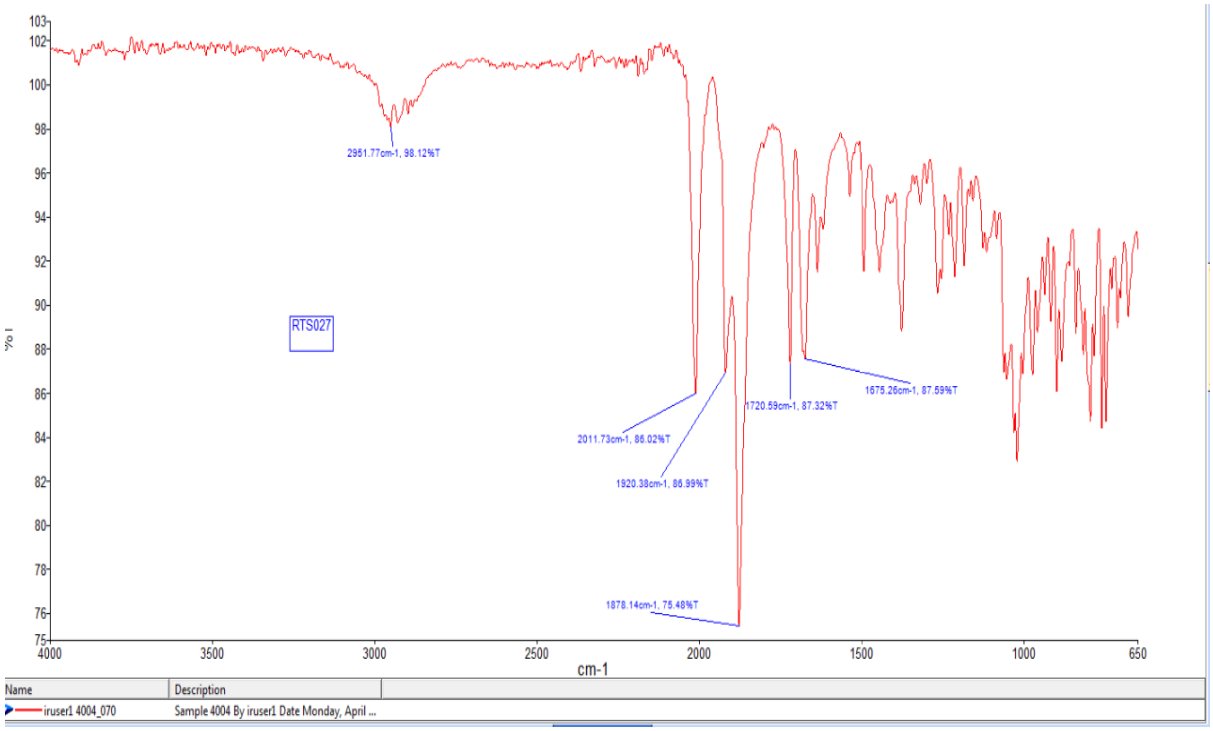
PROTON_01



153


PROTON_01
156
6.74 6.73 6.73 6.73 6.72 6.72 6.20 6.20 5.59 4.30 4.30 4.29 4.11 4.09 4.06 4.06 4.05 4.05 4.02 4.00 3.38 3.38 3.38 3.37 3.37 2.68 2.67 2.66 2.65 2.64 1.89 1.21
I (dd) 4.06 J(5.7, 1.0)
B (d) 6.20 J(1.2)
G (d) 4.01 J(9.8)
L (d) 2.65 J(5.7)
A (dt) 6.73 J(6.4, 1.6)
C (s) 5.59
F (d) 4.10 J(9.8)
K (d) 2.67 J(4.1)
D (s) 1.89
E (s) 1.21
J (dd) 3.38 J(5.8, 1.3)
H (m) 4.29
1.00 1.01 0.36 0.95 1.16 0.99 1.14 1.00 0.60 1.33 1.22 3.38
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800 700 600 500 400 300 200 100 0 -100

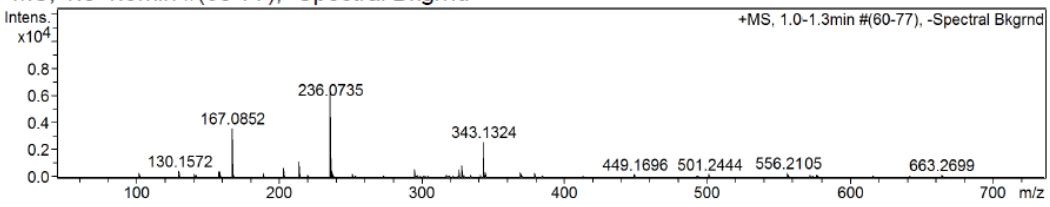

CARBON_01
206.05 191.93 144.65 143.58 134.83 121.19 82.09 78.69 76.31 72.72 51.40 47.12 43.08 34.59 15.88 15.38
156
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



Confirmation of Expected Formula

Sample-ID	sl_rs755_RTS027	Submitter	rs755 Ryan Stendall
Analysis Name	sl_rs755_RTS027_351681_40_01_57081.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	03/04/2017 17:12:53
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	130.1572	476	8.4	12	887.7
2	167.0852	3613	63.5	86	4036.9
3	203.0590	648	11.4	13	630.7
4	214.0930	1134	19.9	27	1000.5
5	236.0735	5686	100.0	192	4098.1
6	237.0800	434	7.6	17	310.0
7	295.0976	622	10.9	31	309.4
8	326.1347	598	10.5	14	239.8
9	328.3572	868	15.3	55	343.3
10	343.1324	2591	45.6	173	936.5

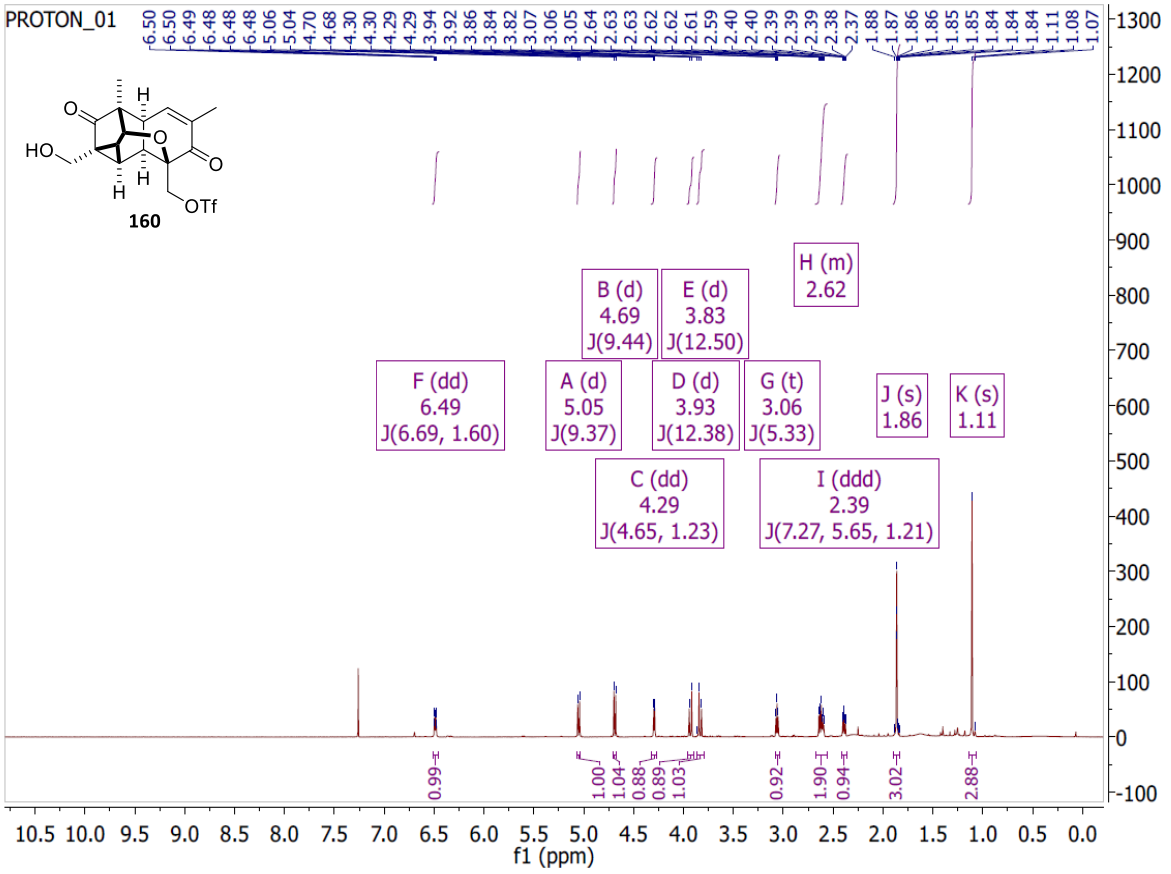
Generate Molecular Formula Parameters

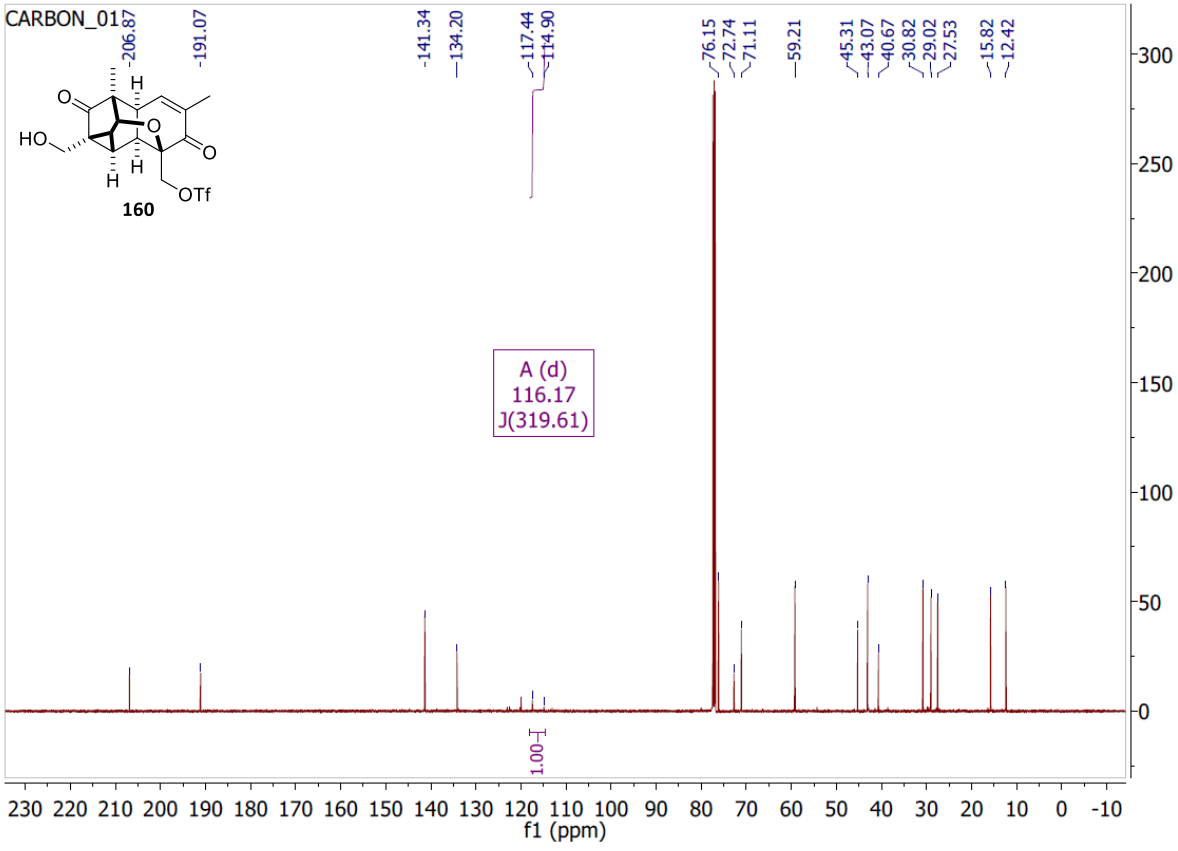
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

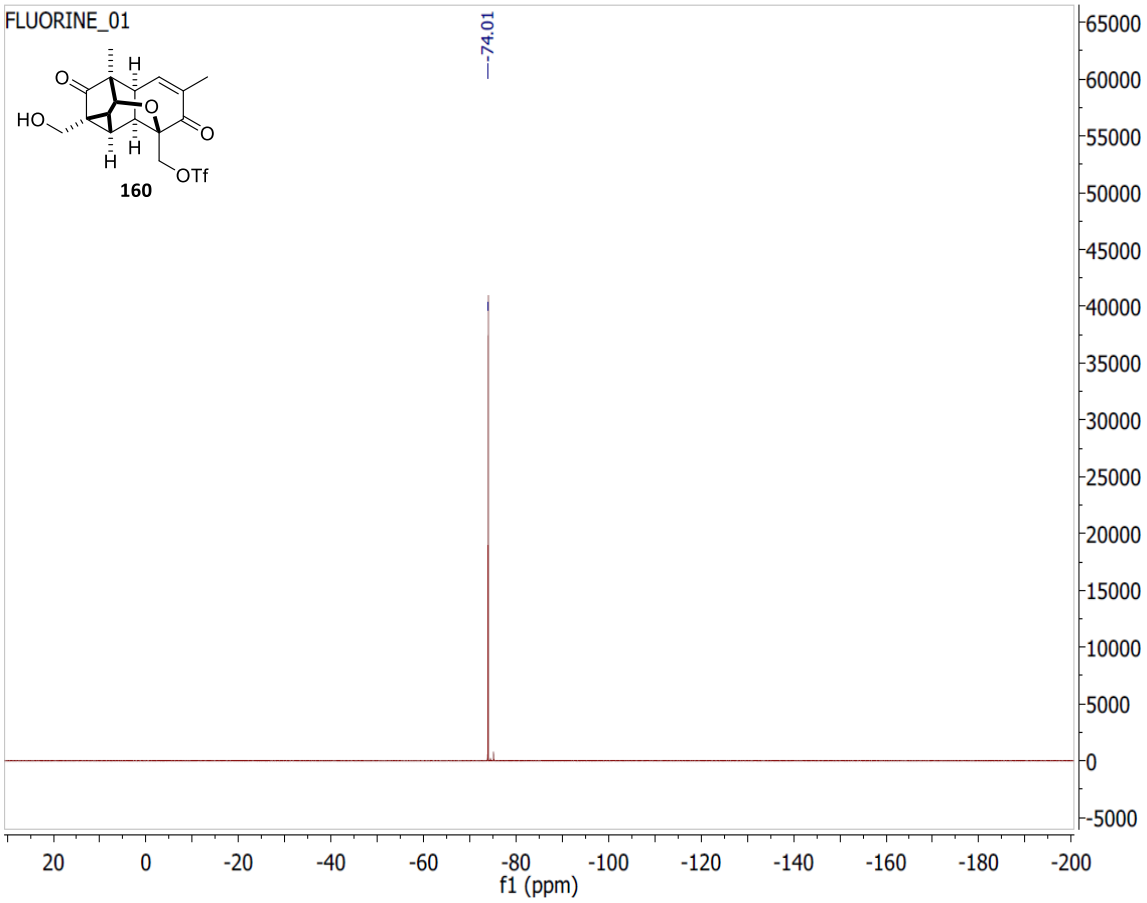
Expected Formula C15 H14 O3 **Adduct(s):** H, Na

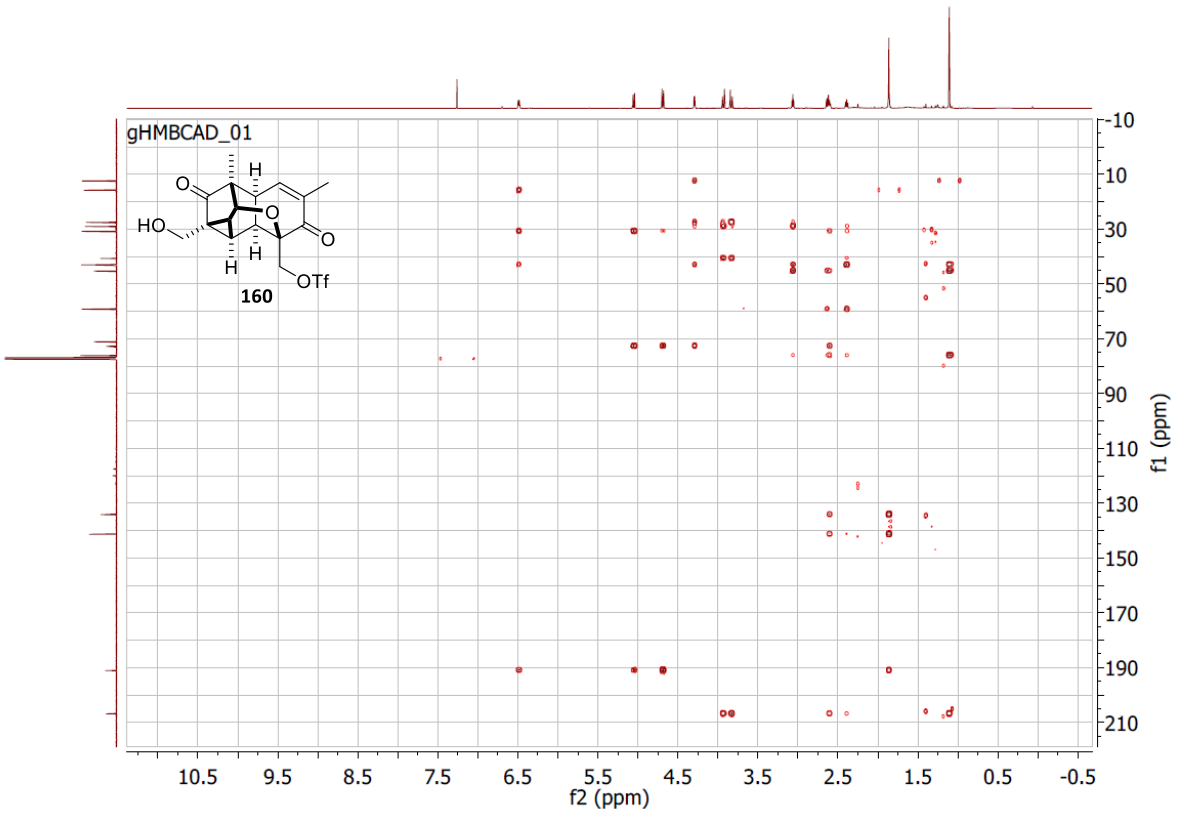
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula

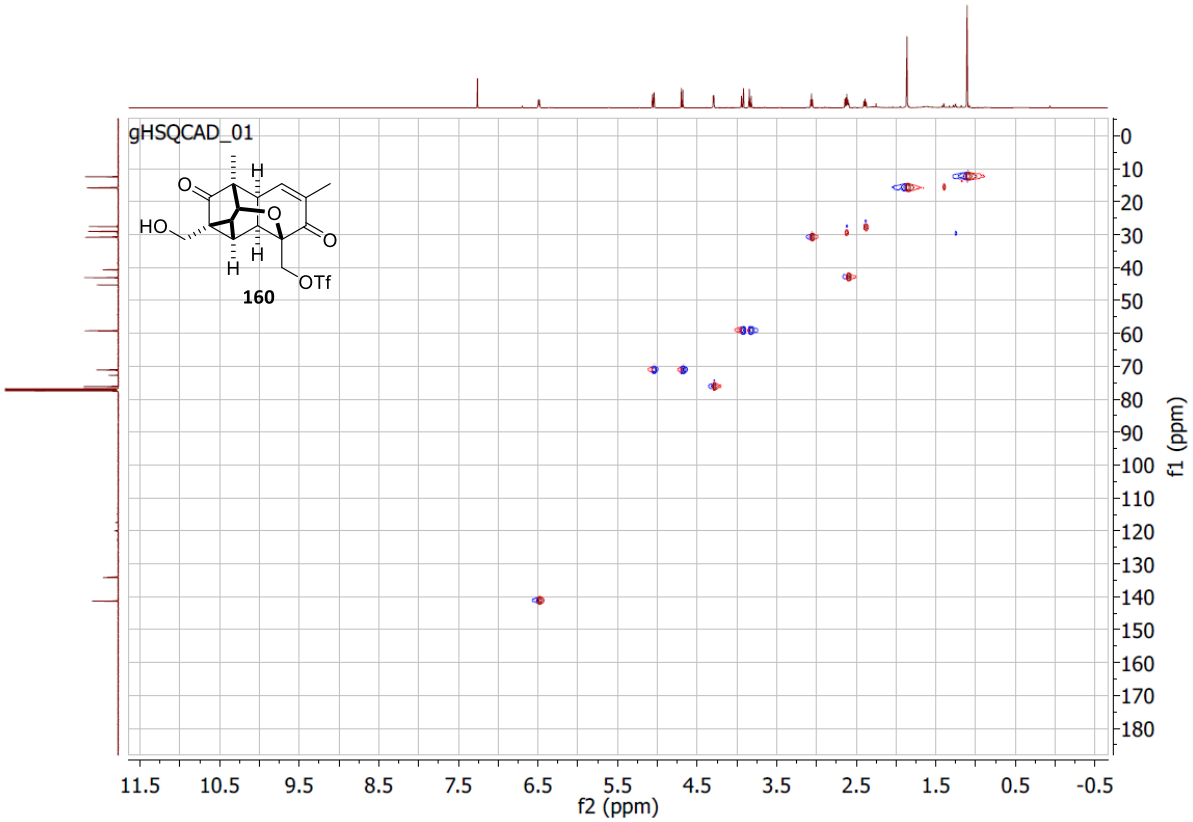
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

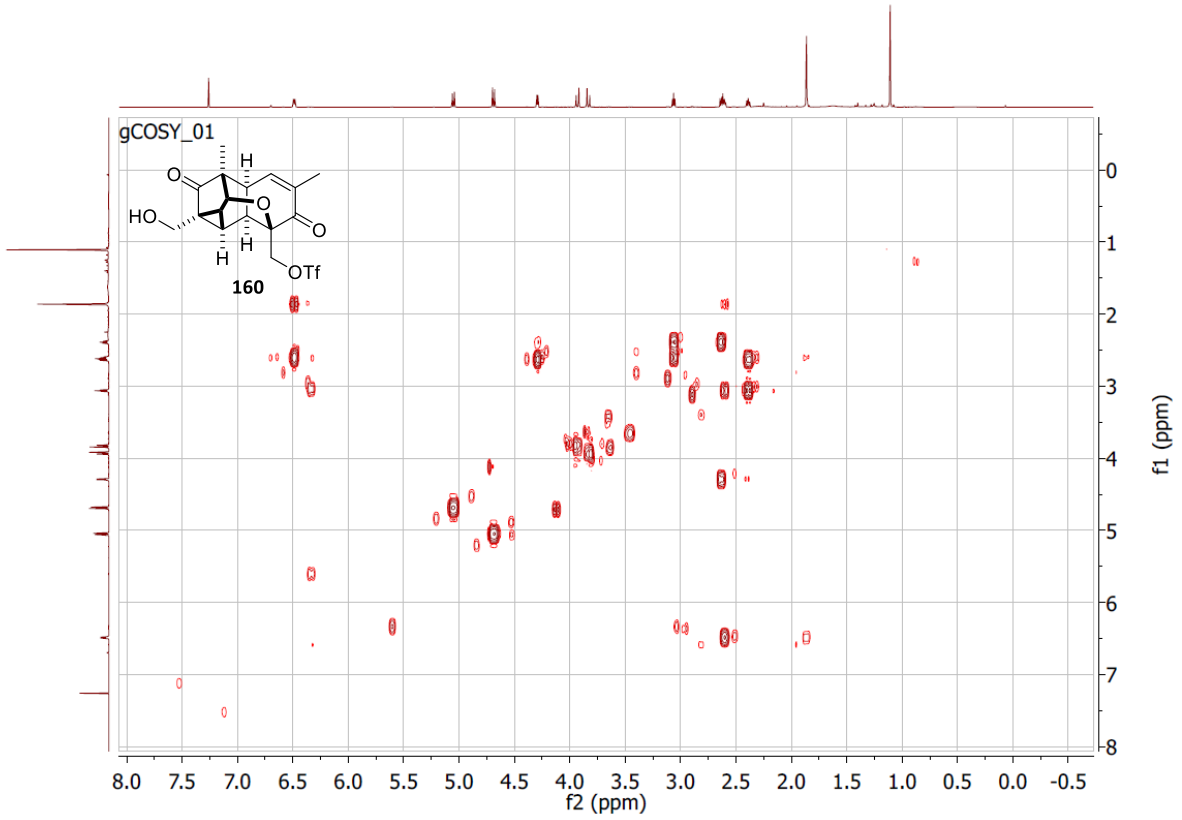

PROTON_01
160
H (m)
2.62
B (d)
4.69
J(9.44)
E (d)
3.83
J(12.50)
F (dd)
6.49
J(6.69, 1.60)
A (d)
5.05
J(9.37)
D (d)
3.93
J(12.38)
G (t)
3.06
J(5.33)
J (s)
1.86
K (s)
1.11
C (dd)
4.29
J(4.65, 1.23)
I (ddd)
2.39
J(7.27, 5.65, 1.21)
f1 (ppm)

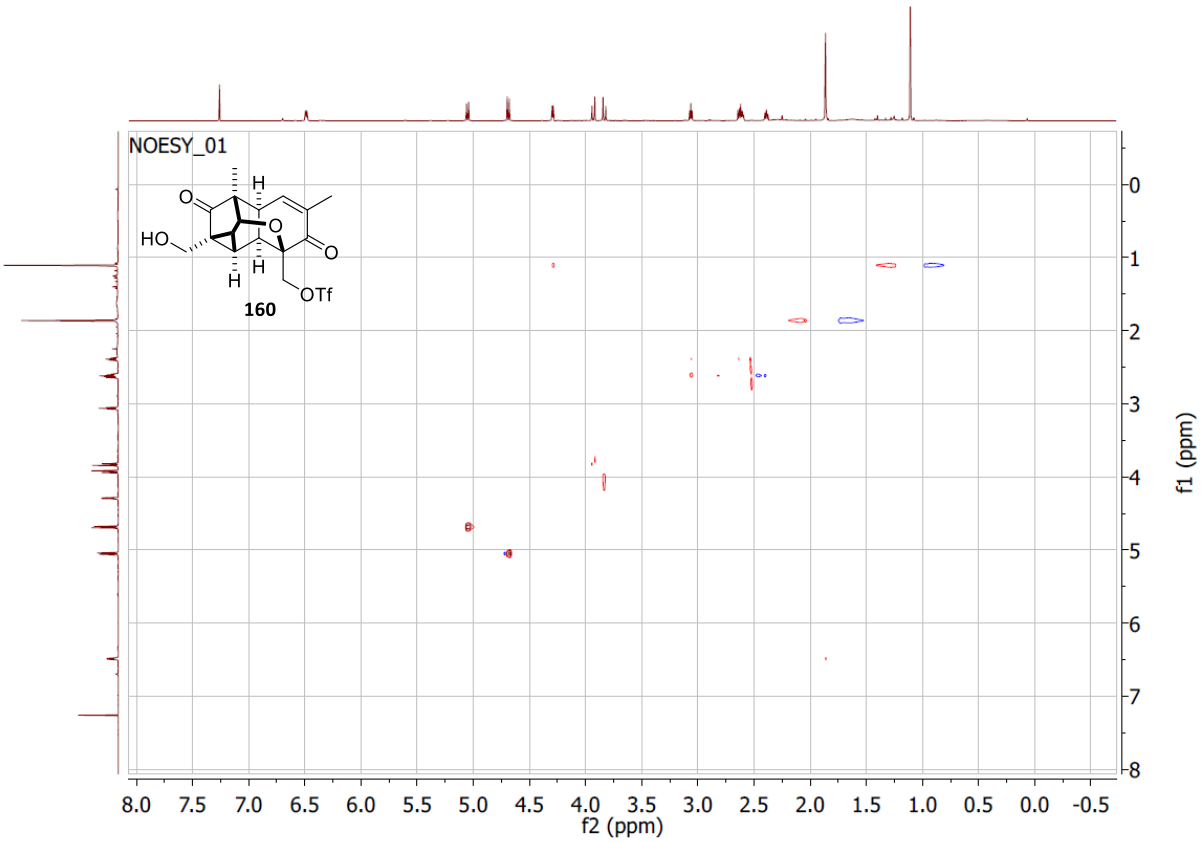

CARBON_01
160
A (d)
116.17
J(319.61)
f1 (ppm)

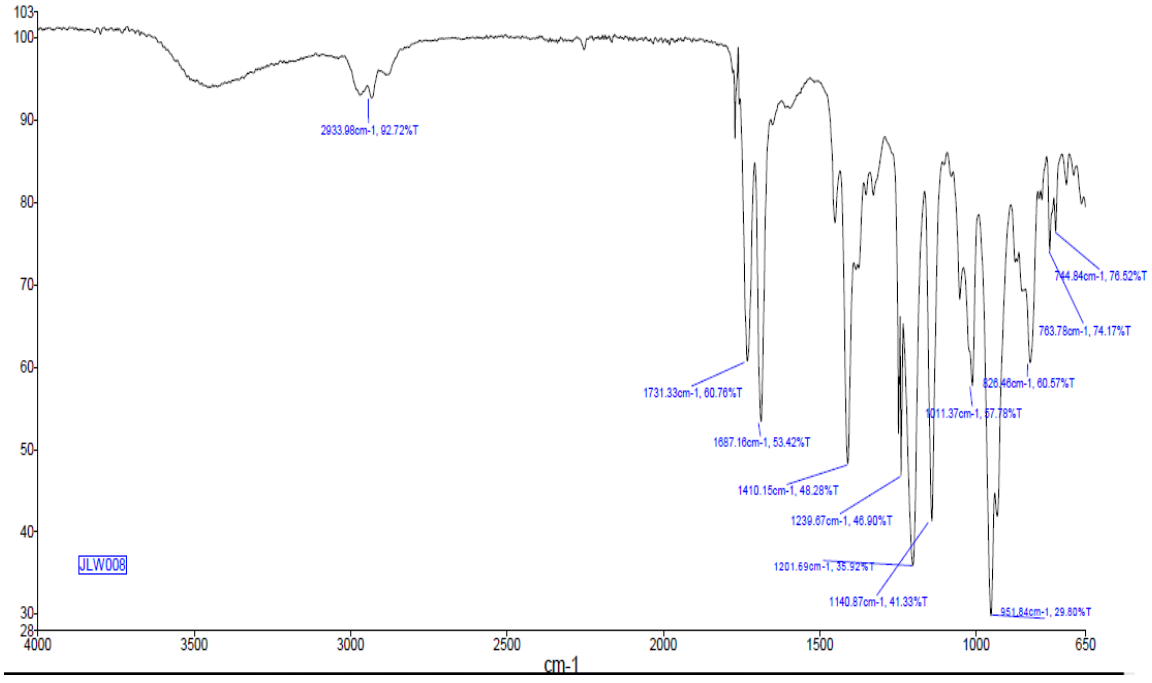

FLUORINE_01
-74.01
160
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)


gHMBCAD_01
160
-10
10
30
50
70
90
110
130
150
170
190
210
f1 (ppm)
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f2 (ppm)


gHSQCAD_01
HO
O
O
O
H
H
H
OTf
160
f2 (ppm)
f1 (ppm)


gCOSY_01
HO
O
O
O
H
H
H
OTf
160
f2 (ppm)
f1 (ppm)

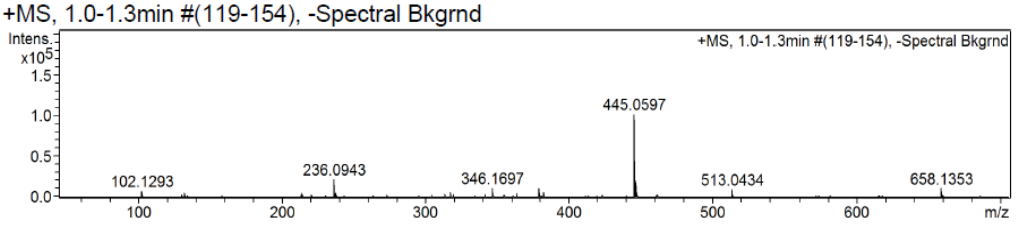

NOESY_01
HO
O
H
O
O
H
H
OTf
160
f2 (ppm)
f1 (ppm)


2933.98cm-1, 92.72%T
1731.33cm-1, 60.76%T
1687.16cm-1, 53.42%T
1410.15cm-1, 48.28%T
1239.67cm-1, 46.90%T
1201.69cm-1, 35.92%T
1140.87cm-1, 41.33%T
951.84cm-1, 29.80%T
1011.37cm-1, 57.78%T
826.46cm-1, 60.57%T
763.78cm-1, 74.17%T
744.84cm-1, 76.52%T
JLW008
cm-1

Confirmation of Expected Formula

Sample-ID	ba_sel_JLW008	Submitter	bea23 Ben Alexander
Analysis Name	ba_sel_JLW008_352377_11_01_57880.d	Supervisor	sl288 Simon Lewis
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	17/07/2017 16:17:06
Ionisation Mode	positive electrospray (ESI)		

+MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	102.1293	7756	7.6	184	4315.3
2	236.0943	21600	21.3	232	1216.5
3	316.9296	6615	6.5	352	251.6
4	346.1697	11327	11.1	714	361.7
5	379.1161	10655	10.5	706	331.9
6	382.1258	6357	6.3	401	203.4
7	445.0597	101635	100.0	7510	3445.4
8	446.0594	20984	20.6	1356	703.2
9	513.0434	9781	9.6	828	576.5
10	658.1353	10913	10.7	1249	554.2

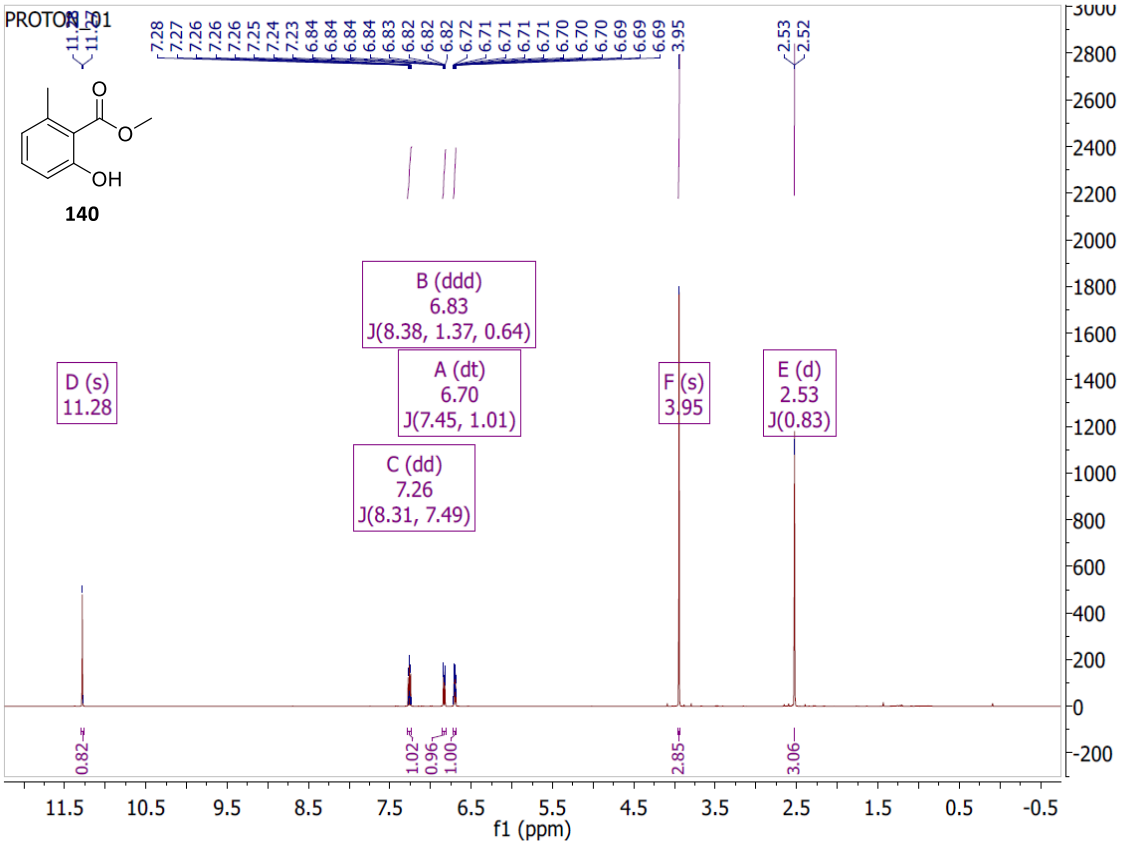
Generate Molecular Formula Parameters

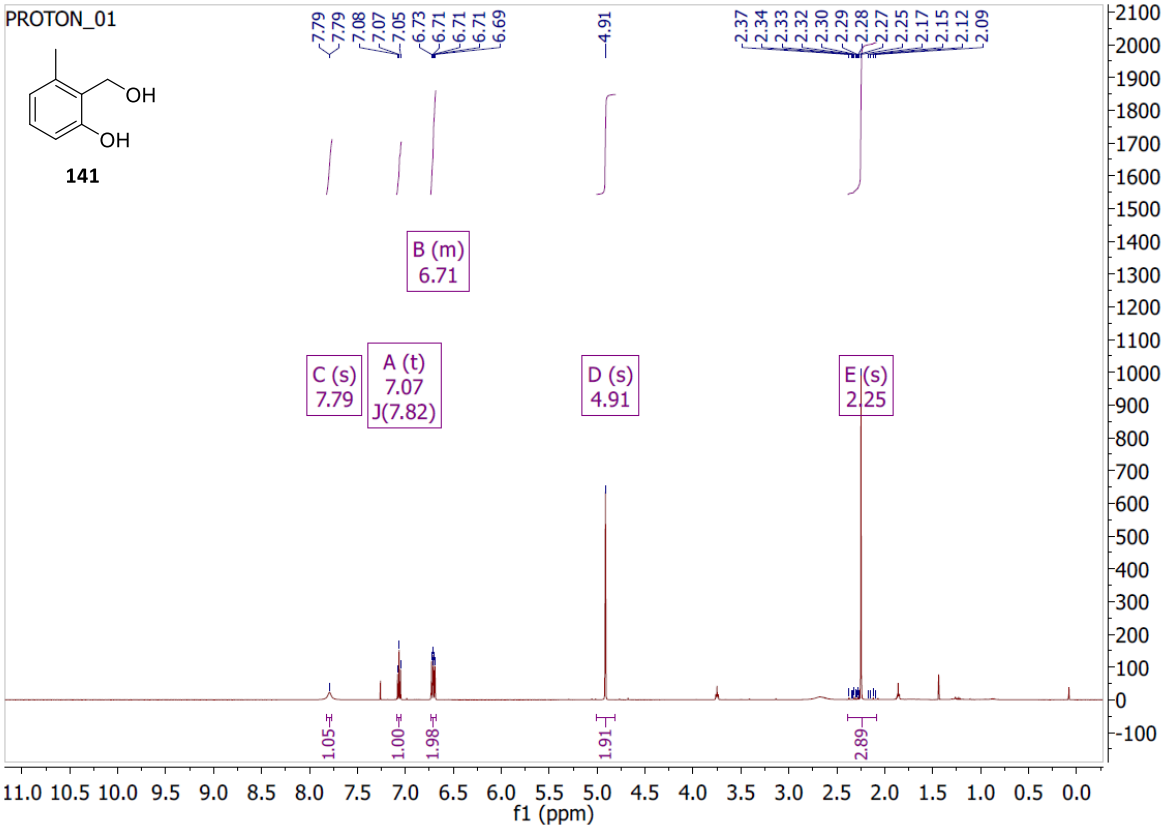
Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

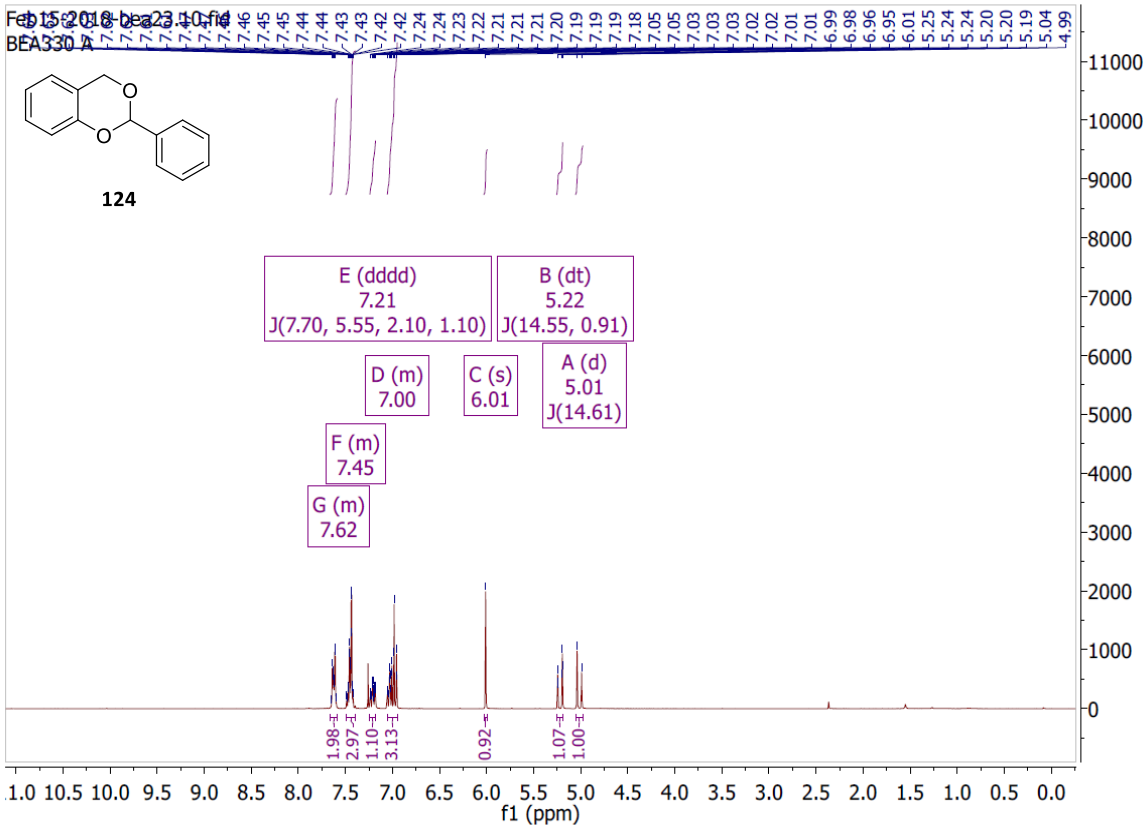
Expected Formula C17 H17 F3 O7 S1 **Adduct(s):** H, Na

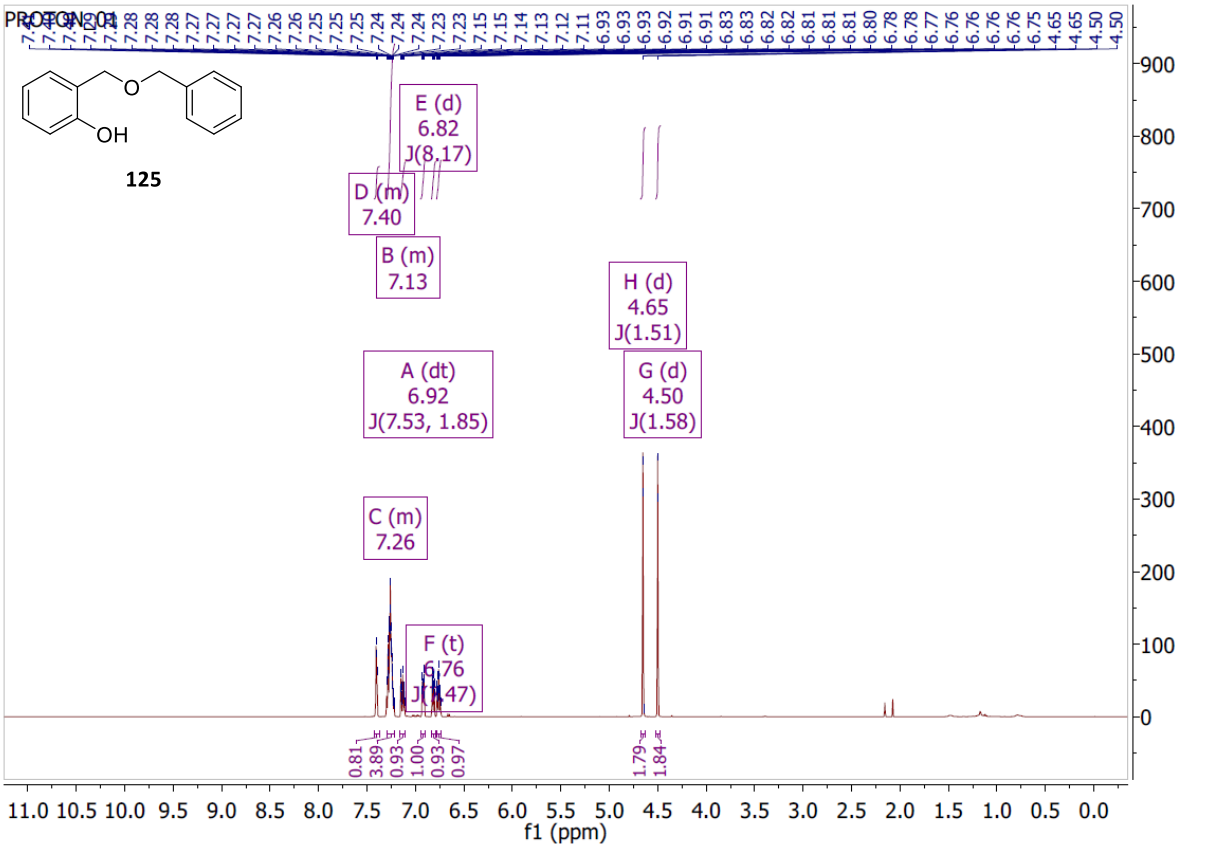
#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	423.0726	423.0720	1.50	0.0231	C 17 H 18 F 3 O 7 S 1

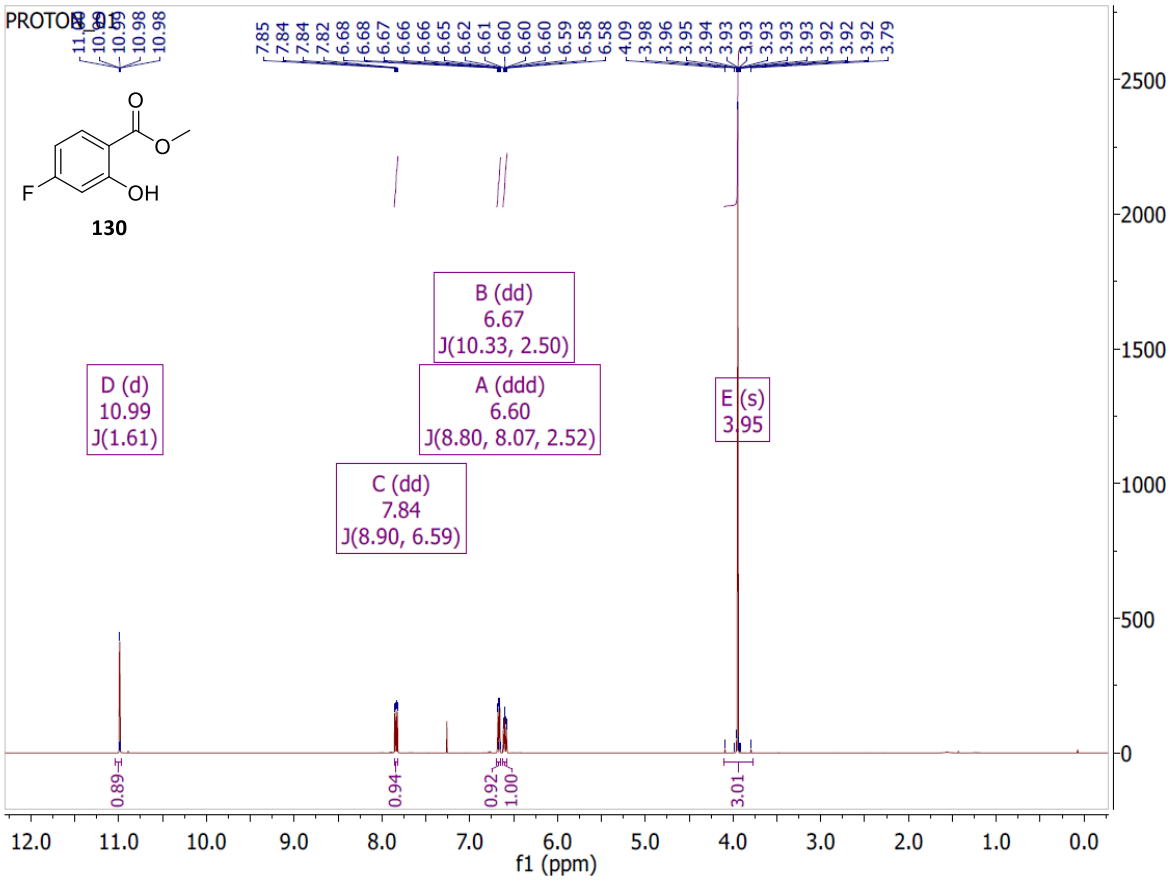
Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication

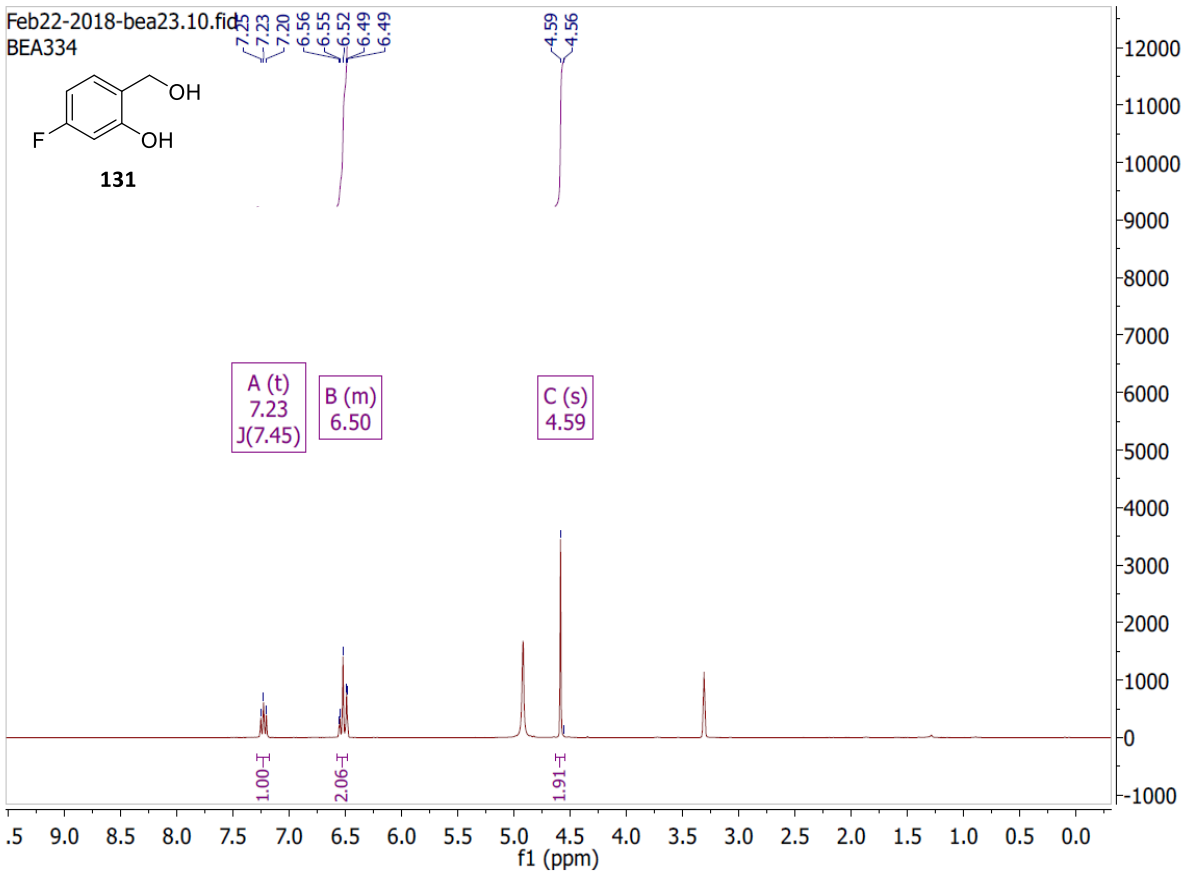



PROTON_01
OH
OH
141
B (m)
6.71
C (s)
7.79
A (t)
7.07
J(7.82)
D (s)
4.91
E (s)
2.25
f1 (ppm)


BEA330 A
124
E (dddd)
7.21
J(7.70, 5.55, 2.10, 1.10)
B (dt)
5.22
J(14.55, 0.91)
D (m)
7.00
C (s)
6.01
A (d)
5.01
J(14.61)
F (m)
7.45
G (m)
7.62
f1 (ppm)


PROTON_01
125
E (d)
6.82
J(8,17)
D (m)
7.40
B (m)
7.13
H (d)
4.65
J(1.51)
A (dt)
6.92
J(7.53, 1.85)
G (d)
4.50
J(1.58)
C (m)
7.26
F (t)
6.76
f1 (ppm)


130
B (dd)
6.67
J(10.33, 2.50)
D (d)
10.99
J(1.61)
A (ddd)
6.60
J(8.80, 8.07, 2.52)
E (s)
3.95
C (dd)
7.84
J(8.90, 6.59)
f1 (ppm)


Feb22-2018-bea23.10.fid
BEA334
OH
F
OH
131
7.25
7.23
7.20
6.56
6.55
6.52
6.49
6.49
4.59
4.56
A (t)
7.23
J(7.45)
B (m)
6.50
C (s)
4.59
1.00
2.06
1.91
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

7.2: X-ray crystal structure data

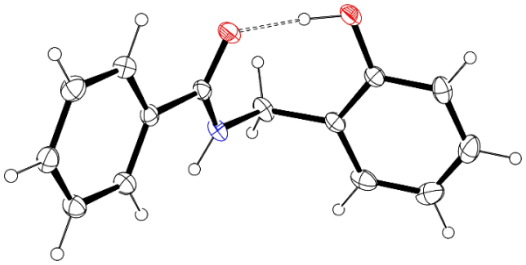


Table 1. Crystal data and structure refinement for k15sel3.

Identification code	k15sel3	
Empirical formula	C14 H13 N O2	
Formula weight	227.25	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 6.32110(10) Å	α= 90°.
	b = 16.1258(3) Å	β= 93.0565(9)°.
	c = 11.1604(3) Å	γ = 90°.
Volume	1135.99(4) $Å^3$	
Z	4	
Density (calculated)	1.329 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	480	
Crystal size	0.500 x 0.400 x 0.250 mm^3	
Theta range for data collection	3.656 to 27.531°.	
Index ranges	-8<=h<=8, -20<=k<=20, -14<=l<=14	
Reflections collected	17829	
Independent reflections	2600 [R(int) = 0.0366]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.978 and 0.909	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2600 / 0 / 162	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.1079	
R indices (all data)	R1 = 0.0516, wR2 = 0.1137	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.190 and -0.205 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k15sel3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N	608(2)	3056(1)	1195(1)	29(1)
O(1)	6133(1)	3016(1)	1751(1)	38(1)
O(2)	3357(1)	3176(1)	-5(1)	36(1)
C(1)	5192(2)	3237(1)	2781(1)	28(1)
C(2)	6399(2)	3689(1)	3630(1)	36(1)
C(3)	5574(3)	3904(1)	4701(1)	46(1)
C(4)	3541(3)	3665(1)	4944(1)	50(1)
C(5)	2327(2)	3215(1)	4095(1)	40(1)
C(6)	3123(2)	3004(1)	2998(1)	27(1)
C(7)	1764(2)	2526(1)	2081(1)	32(1)
C(8)	1478(2)	3329(1)	209(1)	27(1)
C(9)	153(2)	3844(1)	-659(1)	26(1)
C(10)	-1822(2)	4157(1)	-406(1)	31(1)
C(11)	-2955(2)	4646(1)	-1241(1)	35(1)
C(12)	-2127(2)	4829(1)	-2328(1)	35(1)
C(13)	-160(2)	4522(1)	-2589(1)	38(1)
C(14)	978(2)	4030(1)	-1760(1)	33(1)

Table 3. Bond lengths [Å] for k15sel3.

N-C(8)	1.3306(15)
N-C(7)	1.4717(15)
N-H	0.934(17)
O(1)-C(1)	1.3688(15)
O(1)-H(1)	0.96(2)
O(2)-C(8)	1.2489(14)
C(1)-C(2)	1.3908(17)
C(1)-C(6)	1.3945(16)
C(2)-C(3)	1.374(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.391(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3909(18)
C(5)-H(5)	0.9500
C(6)-C(7)	1.5118(17)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.4978(16)
C(9)-C(10)	1.3892(16)
C(9)-C(14)	1.3931(17)
C(10)-C(11)	1.3897(17)
C(10)-H(10)	0.9500
C(11)-C(12)	1.3787(19)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3840(19)
C(12)-H(12)	0.9500
C(13)-C(14)	1.3887(18)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500

Table 4. Bond lengths [Å] and angles [°] for k15sel3.

C(8)-N-C(7)	122.39(10)
C(8)-N-H	120.7(10)
C(7)-N-H	116.3(10)
C(1)-O(1)-H(1)	109.5(12)
O(1)-C(1)-C(2)	117.44(11)
O(1)-C(1)-C(6)	121.96(11)
C(2)-C(1)-C(6)	120.58(12)
C(3)-C(2)-C(1)	120.34(13)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	120.03(14)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	119.74(13)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	121.06(13)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	118.22(12)
C(5)-C(6)-C(7)	120.14(11)
C(1)-C(6)-C(7)	121.63(11)
N-C(7)-C(6)	113.69(10)
N-C(7)-H(7A)	108.8
C(6)-C(7)-H(7A)	108.8
N-C(7)-H(7B)	108.8
C(6)-C(7)-H(7B)	108.8
H(7A)-C(7)-H(7B)	107.7
O(2)-C(8)-N	122.14(11)
O(2)-C(8)-C(9)	119.38(11)
N-C(8)-C(9)	118.48(10)
C(10)-C(9)-C(14)	118.93(11)
C(10)-C(9)-C(8)	123.18(11)
C(14)-C(9)-C(8)	117.88(10)
C(9)-C(10)-C(11)	120.43(12)
C(9)-C(10)-H(10)	119.8

C(11)-C(10)-H(10)	119.8
C(12)-C(11)-C(10)	120.32(12)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	119.73(12)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	120.23(12)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(13)-C(14)-C(9)	120.35(12)
C(13)-C(14)-H(14)	119.8
C(9)-C(14)-H(14)	119.8

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k15sel3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N	20(1)	30(1)	37(1)	6(1)	-3(1)	-1(1)
O(1)	21(1)	59(1)	34(1)	0(1)	2(1)	0(1)
O(2)	24(1)	46(1)	37(1)	1(1)	1(1)	5(1)
C(1)	26(1)	27(1)	30(1)	6(1)	0(1)	2(1)
C(2)	34(1)	32(1)	42(1)	7(1)	-12(1)	-2(1)
C(3)	59(1)	38(1)	38(1)	-2(1)	-20(1)	13(1)
C(4)	65(1)	60(1)	26(1)	4(1)	0(1)	30(1)
C(5)	33(1)	50(1)	36(1)	17(1)	6(1)	14(1)
C(6)	24(1)	25(1)	32(1)	8(1)	-1(1)	4(1)
C(7)	25(1)	28(1)	44(1)	11(1)	-4(1)	-3(1)
C(8)	22(1)	25(1)	33(1)	-4(1)	-2(1)	-1(1)
C(9)	25(1)	23(1)	30(1)	-2(1)	-3(1)	-2(1)
C(10)	29(1)	32(1)	33(1)	3(1)	1(1)	2(1)
C(11)	32(1)	34(1)	39(1)	1(1)	-2(1)	7(1)
C(12)	44(1)	27(1)	32(1)	0(1)	-7(1)	5(1)
C(13)	45(1)	39(1)	29(1)	2(1)	3(1)	1(1)
C(14)	31(1)	36(1)	34(1)	-2(1)	2(1)	2(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for k15sel3.

	x	y	z	U(eq)
H	-830(30)	3132(10)	1301(14)	45(4)
H(1)	5090(30)	3001(12)	1097(19)	70(6)
H(2)	7802	3849	3469	44
H(3)	6400	4217	5274	55
H(4)	2975	3806	5689	60
H(5)	933	3050	4267	48
H(7A)	2678	2139	1652	39
H(7B)	728	2189	2504	39
H(10)	-2400	4036	342	38
H(11)	-4308	4855	-1061	42
H(12)	-2903	5166	-2895	42
H(13)	414	4647	-3337	45
H(14)	2326	3820	-1946	40

Table 7. Torsion angles [°] for k15sel3.

O(1)-C(1)-C(2)-C(3)	-177.70(11)
C(6)-C(1)-C(2)-C(3)	0.74(18)
C(1)-C(2)-C(3)-C(4)	0.6(2)
C(2)-C(3)-C(4)-C(5)	-0.9(2)
C(3)-C(4)-C(5)-C(6)	-0.2(2)
C(4)-C(5)-C(6)-C(1)	1.54(18)
C(4)-C(5)-C(6)-C(7)	-179.12(11)
O(1)-C(1)-C(6)-C(5)	176.58(11)
C(2)-C(1)-C(6)-C(5)	-1.79(17)
O(1)-C(1)-C(6)-C(7)	-2.75(17)
C(2)-C(1)-C(6)-C(7)	178.88(10)
C(8)-N-C(7)-C(6)	84.86(14)
C(5)-C(6)-C(7)-N	94.16(13)
C(1)-C(6)-C(7)-N	-86.52(13)
C(7)-N-C(8)-O(2)	-2.58(18)
C(7)-N-C(8)-C(9)	178.04(10)
O(2)-C(8)-C(9)-C(10)	-169.20(11)
N-C(8)-C(9)-C(10)	10.20(17)
O(2)-C(8)-C(9)-C(14)	9.20(16)
N-C(8)-C(9)-C(14)	-171.40(11)
C(14)-C(9)-C(10)-C(11)	0.22(18)
C(8)-C(9)-C(10)-C(11)	178.60(11)
C(9)-C(10)-C(11)-C(12)	-0.36(19)
C(10)-C(11)-C(12)-C(13)	0.3(2)
C(11)-C(12)-C(13)-C(14)	0.0(2)
C(12)-C(13)-C(14)-C(9)	-0.1(2)
C(10)-C(9)-C(14)-C(13)	0.02(18)
C(8)-C(9)-C(14)-C(13)	-178.44(11)

Table 8. Hydrogen bonds for k15sel3 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N-H...O(1)#1	0.934(17)	2.016(17)	2.9292(14)	165.4(14)
O(1)-H(1)...O(2)	0.96(2)	1.63(2)	2.5731(13)	168.5(19)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z

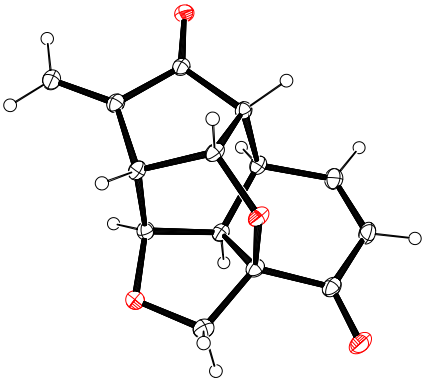


Table 1. Crystal data and structure refinement for s16sel9.

Identification code	s16sel9	
Empirical formula	C14 H12 O4	
Formula weight	244.24	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.54260(10) Å	α= 90°.
	b = 5.78890(10) Å	β= 94.0330(10)°.
	c = 17.7918(2) Å	γ = 90°.
Volume	1083.15(2) $Å^3$	
Z	4	
Density (calculated)	1.498 Mg/m^3	
Absorption coefficient	0.917 mm^{-1}	
F(000)	512	
Crystal size	0.150 x 0.080 x 0.080 mm^3	
Theta range for data collection	4.204 to 73.110°.	
Index ranges	-13<=h<=12, -7<=k<=7, -21<=l<=22	

Reflections collected	20572
Independent reflections	2155 [R(int) = 0.0254]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.71345
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2155 / 0 / 163
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0867
R indices (all data)	R1 = 0.0363, wR2 = 0.0877
Extinction coefficient	n/a
Largest diff. peak and hole	0.286 and -0.226 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s16sel9. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8709(1)	10517(2)	2282(1)	32(1)
O(2)	5023(1)	2226(2)	4280(1)	25(1)
O(3)	7319(1)	9131(1)	3740(1)	21(1)
O(4)	9780(1)	6994(2)	4344(1)	28(1)
C(1)	8136(1)	8905(2)	2538(1)	23(1)
C(2)	7146(1)	7587(2)	2104(1)	28(1)
C(3)	6609(1)	5721(2)	2388(1)	26(1)
C(4)	6967(1)	4714(2)	3156(1)	20(1)
C(5)	6015(1)	5581(2)	3734(1)	20(1)
C(6)	5846(1)	3701(2)	4312(1)	19(1)
C(7)	6865(1)	4014(2)	4926(1)	20(1)
C(8)	7018(1)	2618(2)	5522(1)	24(1)
C(9)	7640(1)	6095(2)	4730(1)	20(1)
C(10)	6702(1)	7498(2)	4202(1)	20(1)
C(11)	8357(1)	8143(2)	3353(1)	19(1)
C(12)	8311(1)	5513(2)	3421(1)	19(1)
C(13)	8751(1)	5355(2)	4259(1)	21(1)
C(14)	9608(1)	8751(2)	3770(1)	25(1)

Table 3. Bond lengths [Å] for s16sel9.

O(1)-C(1)	1.2178(16)
O(2)-C(6)	1.2161(15)
O(3)-C(10)	1.4378(14)
O(3)-C(11)	1.4507(13)
O(4)-C(13)	1.4408(15)
O(4)-C(14)	1.4435(16)
C(1)-C(2)	1.4683(19)
C(1)-C(11)	1.5174(16)
C(2)-C(3)	1.3358(19)
C(2)-H(2)	0.9500
C(3)-C(4)	1.5097(17)
C(3)-H(3)	0.9500
C(4)-C(12)	1.5329(17)
C(4)-C(5)	1.5683(16)
C(4)-H(4)	1.0000
C(5)-C(6)	1.5160(16)
C(5)-C(10)	1.5375(17)
C(5)-H(5)	1.0000
C(6)-C(7)	1.4895(17)
C(7)-C(8)	1.3328(17)
C(7)-C(9)	1.5102(17)
C(8)-H(8A)	0.9500
C(8)-H(8B)	0.9500
C(9)-C(10)	1.5464(16)
C(9)-C(13)	1.5482(16)
C(9)-H(9)	1.0000
C(10)-H(10)	1.0000
C(11)-C(14)	1.5079(17)
C(11)-C(12)	1.5283(16)
C(12)-C(13)	1.5326(16)
C(12)-H(12)	1.0000
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900

Table 4. Bond angles [°] for s16sel9.

C(10)-O(3)-C(11)	113.50(9)
C(13)-O(4)-C(14)	109.47(9)
O(1)-C(1)-C(2)	123.60(12)
O(1)-C(1)-C(11)	122.28(12)
C(2)-C(1)-C(11)	114.09(11)
C(3)-C(2)-C(1)	121.71(12)
C(3)-C(2)-H(2)	119.1
C(1)-C(2)-H(2)	119.1
C(2)-C(3)-C(4)	124.70(12)
C(2)-C(3)-H(3)	117.7
C(4)-C(3)-H(3)	117.7
C(3)-C(4)-C(12)	109.18(10)
C(3)-C(4)-C(5)	109.83(10)
C(12)-C(4)-C(5)	108.78(9)
C(3)-C(4)-H(4)	109.7
C(12)-C(4)-H(4)	109.7
C(5)-C(4)-H(4)	109.7
C(6)-C(5)-C(10)	102.96(10)
C(6)-C(5)-C(4)	108.99(9)
C(10)-C(5)-C(4)	106.71(9)
C(6)-C(5)-H(5)	112.5
C(10)-C(5)-H(5)	112.5
C(4)-C(5)-H(5)	112.5
O(2)-C(6)-C(7)	126.48(11)
O(2)-C(6)-C(5)	126.20(11)
C(7)-C(6)-C(5)	107.32(10)
C(8)-C(7)-C(6)	123.40(12)
C(8)-C(7)-C(9)	129.07(12)
C(6)-C(7)-C(9)	107.53(10)
C(7)-C(8)-H(8A)	120.0
C(7)-C(8)-H(8B)	120.0
H(8A)-C(8)-H(8B)	120.0
C(7)-C(9)-C(10)	103.07(10)
C(7)-C(9)-C(13)	110.29(10)

C(10)-C(9)-C(13)	106.97(9)
C(7)-C(9)-H(9)	112.0
C(10)-C(9)-H(9)	112.0
C(13)-C(9)-H(9)	112.0
O(3)-C(10)-C(5)	112.31(10)
O(3)-C(10)-C(9)	113.39(10)
C(5)-C(10)-C(9)	101.94(9)
O(3)-C(10)-H(10)	109.7
C(5)-C(10)-H(10)	109.7
C(9)-C(10)-H(10)	109.7
O(3)-C(11)-C(14)	109.72(10)
O(3)-C(11)-C(1)	105.58(9)
C(14)-C(11)-C(1)	118.17(10)
O(3)-C(11)-C(12)	109.02(9)
C(14)-C(11)-C(12)	103.02(10)
C(1)-C(11)-C(12)	111.17(10)
C(11)-C(12)-C(13)	97.29(10)
C(11)-C(12)-C(4)	108.09(10)
C(13)-C(12)-C(4)	119.41(10)
C(11)-C(12)-H(12)	110.4
C(13)-C(12)-H(12)	110.4
C(4)-C(12)-H(12)	110.4
O(4)-C(13)-C(12)	103.73(9)
O(4)-C(13)-C(9)	110.68(10)
C(12)-C(13)-C(9)	108.76(10)
O(4)-C(13)-H(13)	111.1
C(12)-C(13)-H(13)	111.1
C(9)-C(13)-H(13)	111.1
O(4)-C(14)-C(11)	104.22(10)
O(4)-C(14)-H(14A)	110.9
C(11)-C(14)-H(14A)	110.9
O(4)-C(14)-H(14B)	110.9
C(11)-C(14)-H(14B)	110.9
H(14A)-C(14)-H(14B)	108.9

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s16sel9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	37(1)	31(1)	31(1)	10(1)	10(1)	-3(1)
O(2)	21(1)	25(1)	28(1)	5(1)	3(1)	-2(1)
O(3)	25(1)	16(1)	23(1)	3(1)	10(1)	4(1)
O(4)	22(1)	36(1)	26(1)	8(1)	-2(1)	-5(1)
C(1)	24(1)	23(1)	23(1)	4(1)	8(1)	5(1)
C(2)	31(1)	34(1)	17(1)	6(1)	2(1)	2(1)
C(3)	29(1)	32(1)	18(1)	-1(1)	1(1)	-1(1)
C(4)	24(1)	19(1)	17(1)	1(1)	4(1)	1(1)
C(5)	19(1)	21(1)	20(1)	4(1)	3(1)	3(1)
C(6)	20(1)	20(1)	19(1)	2(1)	5(1)	4(1)
C(7)	22(1)	20(1)	18(1)	0(1)	4(1)	2(1)
C(8)	26(1)	25(1)	20(1)	2(1)	2(1)	1(1)
C(9)	24(1)	20(1)	16(1)	1(1)	3(1)	0(1)
C(10)	23(1)	18(1)	20(1)	2(1)	8(1)	2(1)
C(11)	21(1)	18(1)	20(1)	1(1)	6(1)	3(1)
C(12)	21(1)	17(1)	18(1)	1(1)	5(1)	4(1)
C(13)	20(1)	22(1)	21(1)	3(1)	1(1)	2(1)
C(14)	25(1)	23(1)	26(1)	2(1)	4(1)	-2(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s16sel9.

	x	y	z	U(eq)
H(2)	6882	8074	1607	33
H(3)	5954	4974	2084	32
H(4)	6942	2989	3128	24
H(5)	5188	6111	3483	24
H(8A)	6461	1344	5569	28
H(8B)	7685	2895	5898	28
H(9)	7943	6996	5188	24
H(10)	6081	8322	4507	24
H(12)	8952	4787	3107	23
H(13)	9050	3760	4396	25
H(14A)	10308	8712	3428	29
H(14B)	9572	10307	3998	29

Table 7. Torsion angles [°] for s16sel9.

O(1)-C(1)-C(2)-C(3)	174.81(13)
C(11)-C(1)-C(2)-C(3)	-7.36(18)
C(1)-C(2)-C(3)-C(4)	-2.1(2)
C(2)-C(3)-C(4)-C(12)	-21.47(18)
C(2)-C(3)-C(4)-C(5)	97.73(15)
C(3)-C(4)-C(5)-C(6)	147.12(11)
C(12)-C(4)-C(5)-C(6)	-93.44(11)
C(3)-C(4)-C(5)-C(10)	-102.34(11)
C(12)-C(4)-C(5)-C(10)	17.11(12)
C(10)-C(5)-C(6)-O(2)	153.90(12)
C(4)-C(5)-C(6)-O(2)	-93.07(14)
C(10)-C(5)-C(6)-C(7)	-25.44(11)
C(4)-C(5)-C(6)-C(7)	87.59(11)
O(2)-C(6)-C(7)-C(8)	2.3(2)
C(5)-C(6)-C(7)-C(8)	-178.36(11)
O(2)-C(6)-C(7)-C(9)	-178.56(11)
C(5)-C(6)-C(7)-C(9)	0.78(12)
C(8)-C(7)-C(9)-C(10)	-156.87(13)
C(6)-C(7)-C(9)-C(10)	24.05(12)
C(8)-C(7)-C(9)-C(13)	89.22(15)
C(6)-C(7)-C(9)-C(13)	-89.85(11)
C(11)-O(3)-C(10)-C(5)	-65.59(12)
C(11)-O(3)-C(10)-C(9)	49.32(13)
C(6)-C(5)-C(10)-O(3)	161.26(9)
C(4)-C(5)-C(10)-O(3)	46.56(12)
C(6)-C(5)-C(10)-C(9)	39.57(11)
C(4)-C(5)-C(10)-C(9)	-75.13(11)
C(7)-C(9)-C(10)-O(3)	-160.10(9)
C(13)-C(9)-C(10)-O(3)	-43.80(13)
C(7)-C(9)-C(10)-C(5)	-39.16(11)
C(13)-C(9)-C(10)-C(5)	77.14(11)
C(10)-O(3)-C(11)-C(14)	-100.19(11)
C(10)-O(3)-C(11)-C(1)	131.45(10)
C(10)-O(3)-C(11)-C(12)	11.94(13)
O(1)-C(1)-C(11)-O(3)	100.13(13)
C(2)-C(1)-C(11)-O(3)	-77.74(13)

O(1)-C(1)-C(11)-C(14)	-23.01(18)
C(2)-C(1)-C(11)-C(14)	159.12(11)
O(1)-C(1)-C(11)-C(12)	-141.79(12)
C(2)-C(1)-C(11)-C(12)	40.34(14)
O(3)-C(11)-C(12)-C(13)	-71.85(11)
C(14)-C(11)-C(12)-C(13)	44.65(11)
C(1)-C(11)-C(12)-C(13)	172.18(9)
O(3)-C(11)-C(12)-C(4)	52.39(12)
C(14)-C(11)-C(12)-C(4)	168.89(9)
C(1)-C(11)-C(12)-C(4)	-63.58(12)
C(3)-C(4)-C(12)-C(11)	52.17(13)
C(5)-C(4)-C(12)-C(11)	-67.68(12)
C(3)-C(4)-C(12)-C(13)	161.89(11)
C(5)-C(4)-C(12)-C(13)	42.04(14)
C(14)-O(4)-C(13)-C(12)	25.92(12)
C(14)-O(4)-C(13)-C(9)	-90.57(11)
C(11)-C(12)-C(13)-O(4)	-42.89(11)
C(4)-C(12)-C(13)-O(4)	-158.46(10)
C(11)-C(12)-C(13)-C(9)	74.94(11)
C(4)-C(12)-C(13)-C(9)	-40.63(14)
C(7)-C(9)-C(13)-O(4)	-154.78(10)
C(10)-C(9)-C(13)-O(4)	93.82(11)
C(7)-C(9)-C(13)-C(12)	91.88(12)
C(10)-C(9)-C(13)-C(12)	-19.52(13)
C(13)-O(4)-C(14)-C(11)	3.11(13)
O(3)-C(11)-C(14)-O(4)	85.00(11)
C(1)-C(11)-C(14)-O(4)	-153.96(10)
C(12)-C(11)-C(14)-O(4)	-30.99(12)

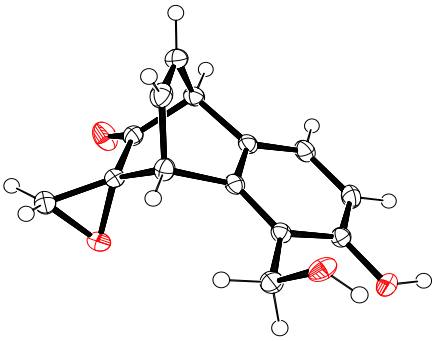


Table 1. Crystal data and structure refinement for s16sel19.

Identification code	s16sel19	
Empirical formula	C14 H12 O4	
Formula weight	244.24	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 9.91860(10) Å	α= 90°.
	b = 9.17150(10) Å	β= 90°.
	c = 25.0459(4) Å	γ = 90°.
Volume	2278.39(5) $Å^3$	
Z	8	
Density (calculated)	1.424 Mg/m^3	
Absorption coefficient	0.872 mm^{-1}	
F(000)	1024	
Crystal size	0.100 x 0.080 x 0.050 mm^3	
Theta range for data collection	3.529 to 73.167°.	
Index ranges	-11<=h<=12, -9<=k<=11, -31<=l<=30	
Reflections collected	15259	
Independent reflections	2263 [R(int) = 0.0319]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.82400	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2263 / 0 / 171	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0870	
R indices (all data)	R1 = 0.0379, wR2 = 0.0893	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.265 and -0.197 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s16sel19. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2818(1)	6824(1)	2719(1)	32(1)
O(2)	2084(1)	7482(1)	3813(1)	23(1)
O(3)	6751(1)	5435(1)	4992(1)	24(1)
O(4)	6271(1)	8557(1)	5210(1)	23(1)
C(1)	3570(1)	7453(1)	3018(1)	20(1)
C(2)	3101(1)	8260(1)	3516(1)	18(1)
C(3)	1732(1)	8840(2)	3552(1)	24(1)
C(4)	4291(1)	8883(1)	3824(1)	19(1)
C(5)	5180(1)	7570(1)	3951(1)	17(1)
C(6)	5549(1)	7089(1)	4456(1)	17(1)
C(7)	5144(1)	7830(1)	4967(1)	21(1)
C(8)	6385(1)	5851(1)	4490(1)	19(1)
C(9)	6807(1)	5112(1)	4035(1)	22(1)
C(10)	6412(1)	5610(1)	3532(1)	21(1)
C(11)	5609(1)	6834(1)	3490(1)	18(1)
C(12)	5108(1)	7506(1)	2972(1)	20(1)
C(13)	5432(1)	9128(2)	2982(1)	24(1)
C(14)	5027(1)	9825(1)	3418(1)	24(1)

Table 3. Bond lengths [Å] for s16sel19.

O(1)-C(1)	1.2052(16)
O(2)-C(2)	1.4426(14)
O(2)-C(3)	1.4488(16)
O(3)-C(8)	1.3638(14)
O(3)-H(3)	0.88(2)
O(4)-C(7)	1.4370(15)
O(4)-H(4A)	0.83(2)
C(1)-C(2)	1.5225(16)
C(1)-C(12)	1.5299(17)
C(2)-C(3)	1.4611(17)
C(2)-C(4)	1.5208(16)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(14)	1.5211(17)
C(4)-C(5)	1.5259(16)
C(4)-H(4)	1.0000
C(5)-C(6)	1.3883(16)
C(5)-C(11)	1.4030(16)
C(6)-C(8)	1.4086(17)
C(6)-C(7)	1.5034(16)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.3895(17)
C(9)-C(10)	1.3966(17)
C(9)-H(9)	0.9500
C(10)-C(11)	1.3810(17)
C(10)-H(10)	0.9500
C(11)-C(12)	1.5219(16)
C(12)-C(13)	1.5218(18)
C(12)-H(12)	1.0000
C(13)-C(14)	1.3273(19)
C(13)-H(13)	0.9500
C(14)-H(14)	0.950

Table 4. Bond angles [°] for s16sel19.

C(2)-O(2)-C(3)	60.70(7)
C(8)-O(3)-H(3)	110.3(12)
C(7)-O(4)-H(4A)	109.2(13)
O(1)-C(1)-C(2)	123.59(11)
O(1)-C(1)-C(12)	125.76(11)
C(2)-C(1)-C(12)	110.60(10)
O(2)-C(2)-C(3)	59.86(8)
O(2)-C(2)-C(4)	117.86(9)
C(3)-C(2)-C(4)	123.55(11)
O(2)-C(2)-C(1)	113.29(10)
C(3)-C(2)-C(1)	120.83(11)
C(4)-C(2)-C(1)	111.10(10)
O(2)-C(3)-C(2)	59.44(8)
O(2)-C(3)-H(3A)	117.8
C(2)-C(3)-H(3A)	117.8
O(2)-C(3)-H(3B)	117.8
C(2)-C(3)-H(3B)	117.8
H(3A)-C(3)-H(3B)	115.0
C(2)-C(4)-C(14)	104.30(9)
C(2)-C(4)-C(5)	104.97(9)
C(14)-C(4)-C(5)	108.14(10)
C(2)-C(4)-H(4)	112.9
C(14)-C(4)-H(4)	112.9
C(5)-C(4)-H(4)	112.9
C(6)-C(5)-C(11)	121.07(11)
C(6)-C(5)-C(4)	126.47(10)
C(11)-C(5)-C(4)	112.46(10)
C(5)-C(6)-C(8)	117.81(11)
C(5)-C(6)-C(7)	124.08(11)
C(8)-C(6)-C(7)	118.09(10)
O(4)-C(7)-C(6)	111.20(10)
O(4)-C(7)-H(7A)	109.4
C(6)-C(7)-H(7A)	109.4
O(4)-C(7)-H(7B)	109.4
C(6)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
O(3)-C(8)-C(9)	122.66(11)
O(3)-C(8)-C(6)	115.92(11)

C(9)-C(8)-C(6)	121.42(11)
C(8)-C(9)-C(10)	119.70(11)
C(8)-C(9)-H(9)	120.2
C(10)-C(9)-H(9)	120.2
C(11)-C(10)-C(9)	119.73(11)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(10)-C(11)-C(5)	120.27(11)
C(10)-C(11)-C(12)	125.58(11)
C(5)-C(11)-C(12)	114.14(10)
C(13)-C(12)-C(11)	108.17(10)
C(13)-C(12)-C(1)	103.94(10)
C(11)-C(12)-C(1)	104.30(9)
C(13)-C(12)-H(12)	113.2
C(11)-C(12)-H(12)	113.2
C(1)-C(12)-H(12)	113.2
C(14)-C(13)-C(12)	114.89(11)
C(14)-C(13)-H(13)	122.6
C(12)-C(13)-H(13)	122.6
C(13)-C(14)-C(4)	114.91(11)
C(13)-C(14)-H(14)	122.5
C(4)-C(14)-H(14)	122.5

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s16sel19. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	49(1)	27(1)	-14(1)	-5(1)	1(1)
O(2)	20(1)	28(1)	21(1)	3(1)	4(1)	-1(1)
O(3)	24(1)	27(1)	21(1)	5(1)	-3(1)	5(1)
O(4)	32(1)	20(1)	17(1)	2(1)	-5(1)	-6(1)
C(1)	19(1)	24(1)	16(1)	1(1)	-1(1)	2(1)
C(2)	18(1)	20(1)	16(1)	2(1)	0(1)	1(1)
C(3)	20(1)	31(1)	23(1)	2(1)	0(1)	5(1)
C(4)	20(1)	19(1)	18(1)	-2(1)	-2(1)	3(1)
C(5)	14(1)	17(1)	19(1)	-1(1)	-1(1)	-2(1)
C(6)	14(1)	18(1)	18(1)	-1(1)	-1(1)	-2(1)
C(7)	20(1)	24(1)	18(1)	-2(1)	-1(1)	0(1)
C(8)	16(1)	21(1)	20(1)	4(1)	-2(1)	-2(1)
C(9)	17(1)	22(1)	28(1)	0(1)	0(1)	5(1)
C(10)	17(1)	24(1)	22(1)	-4(1)	2(1)	2(1)
C(11)	13(1)	22(1)	18(1)	-1(1)	0(1)	-2(1)
C(12)	17(1)	27(1)	16(1)	0(1)	1(1)	1(1)
C(13)	20(1)	29(1)	24(1)	9(1)	-1(1)	-2(1)
C(14)	22(1)	20(1)	30(1)	4(1)	-5(1)	-2(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s16sel19.

	x	y	z	U(eq)
H(3)	7350(20)	4720(20)	4977(7)	37(5)
H(4A)	6612(19)	8010(20)	5439(8)	36(5)
H(3A)	1584	9707	3780	29
H(3B)	1158	8791	3230	29
H(4)	4012	9437	4149	23
H(7A)	4425	8550	4892	25
H(7B)	4777	7097	5218	25
H(9)	7361	4271	4067	27
H(10)	6696	5109	3220	25
H(12)	5458	7000	2646	24
H(13)	5891	9604	2698	29
H(14)	5184	10836	3472	29

Table 7. Torsion angles [°] for s16sel19.

C(3)-O(2)-C(2)-C(4)	114.58(12)
C(3)-O(2)-C(2)-C(1)	-113.27(12)
O(1)-C(1)-C(2)-O(2)	42.13(17)
C(12)-C(1)-C(2)-O(2)	-135.50(10)
O(1)-C(1)-C(2)-C(3)	-25.56(19)
C(12)-C(1)-C(2)-C(3)	156.82(11)
O(1)-C(1)-C(2)-C(4)	177.49(12)
C(12)-C(1)-C(2)-C(4)	-0.13(13)
C(4)-C(2)-C(3)-O(2)	-105.27(12)
C(1)-C(2)-C(3)-O(2)	100.72(12)
O(2)-C(2)-C(4)-C(14)	-170.97(10)
C(3)-C(2)-C(4)-C(14)	-100.29(13)
C(1)-C(2)-C(4)-C(14)	55.92(12)
O(2)-C(2)-C(4)-C(5)	75.41(12)
C(3)-C(2)-C(4)-C(5)	146.08(11)
C(1)-C(2)-C(4)-C(5)	-57.71(12)
C(2)-C(4)-C(5)-C(6)	-120.40(12)
C(14)-C(4)-C(5)-C(6)	128.71(12)
C(2)-C(4)-C(5)-C(11)	58.93(12)
C(14)-C(4)-C(5)-C(11)	-51.97(13)
C(11)-C(5)-C(6)-C(8)	0.97(17)
C(4)-C(5)-C(6)-C(8)	-179.76(11)
C(11)-C(5)-C(6)-C(7)	179.20(11)
C(4)-C(5)-C(6)-C(7)	-1.53(19)
C(5)-C(6)-C(7)-O(4)	-108.14(13)
C(8)-C(6)-C(7)-O(4)	70.09(14)
C(5)-C(6)-C(8)-O(3)	178.49(10)
C(7)-C(6)-C(8)-O(3)	0.15(16)
C(5)-C(6)-C(8)-C(9)	-1.37(18)
C(7)-C(6)-C(8)-C(9)	-179.71(11)
O(3)-C(8)-C(9)-C(10)	-179.00(11)
C(6)-C(8)-C(9)-C(10)	0.86(19)
C(8)-C(9)-C(10)-C(11)	0.09(19)
C(9)-C(10)-C(11)-C(5)	-0.48(18)
C(9)-C(10)-C(11)-C(12)	179.68(11)
C(6)-C(5)-C(11)-C(10)	-0.07(18)

C(4)-C(5)-C(11)-C(10)	-179.43(11)
C(6)-C(5)-C(11)-C(12)	179.79(10)
C(4)-C(5)-C(11)-C(12)	0.43(14)
C(10)-C(11)-C(12)-C(13)	-129.30(13)
C(5)-C(11)-C(12)-C(13)	50.85(13)
C(10)-C(11)-C(12)-C(1)	120.50(13)
C(5)-C(11)-C(12)-C(1)	-59.35(13)
O(1)-C(1)-C(12)-C(13)	126.52(14)
C(2)-C(1)-C(12)-C(13)	-55.92(12)
O(1)-C(1)-C(12)-C(11)	-120.22(14)
C(2)-C(1)-C(12)-C(11)	57.34(12)
C(11)-C(12)-C(13)-C(14)	-51.26(14)
C(1)-C(12)-C(13)-C(14)	59.18(13)
C(12)-C(13)-C(14)-C(4)	-0.93(16)
C(2)-C(4)-C(14)-C(13)	-57.96(13)
C(5)-C(4)-C(14)-C(13)	53.38(14)

Table 8. Hydrogen bonds for s16sel19 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(4)#1	0.88(2)	1.83(2)	2.6672(13)	157.1(17)
O(4)-H(4A)...O(2)#2	0.83(2)	1.98(2)	2.7476(13)	152.0(18)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y-1/2,z #2 x+1/2,-y+3/2,-z+1

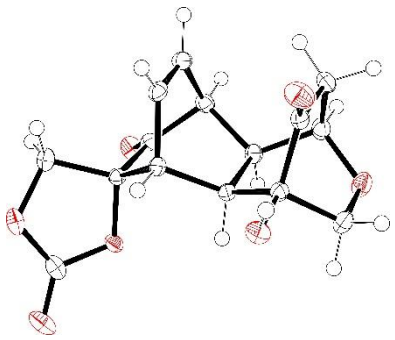


Table 1. Crystal data and structure refinement for s17sel12.

Identification code	s17sel12

Empirical formula	C15 H14 O7	
Formula weight	306.26	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.0103(2) Å	α= 90°.
	b = 10.83020(10) Å	β= 103.155(2)°.
	c = 10.8212(2) Å	γ = 90°.
Volume	1256.50(4) $Å^3$	
Z	4	
Density (calculated)	1.619 Mg/m^3	
Absorption coefficient	1.110 mm^{-1}	
F(000)	640	
Crystal size	0.200 x 0.200 x 0.050 mm^3	
Theta range for data collection	4.123 to 73.151°.	
Index ranges	-13<=h<=13, -13<=k<=10, -12<=l<=13	
Reflections collected	14877	
Independent reflections	2509 [R(int) = 0.0305]	
Completeness to theta = 1.000°	0.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86486	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2509 / 0 / 203	
Goodness-of-fit on F^2	1.111	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1004	
R indices (all data)	R1 = 0.0407, wR2 = 0.1019	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.302 and -0.244 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17sel12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7248(1)	4190(1)	2958(1)	28(1)
C(1)	6335(1)	4791(1)	2546(2)	19(1)
O(2)	5441(1)	4998(1)	3197(1)	17(1)
C(2)	4990(2)	6127(2)	1338(2)	19(1)
O(3)	6047(1)	5317(1)	1401(1)	22(1)
C(3)	4393(1)	5619(1)	2375(1)	14(1)
O(4)	4666(1)	7391(1)	3751(1)	24(1)
C(4)	3951(1)	6645(1)	3165(1)	16(1)
O(5)	45(1)	3301(1)	1122(1)	28(1)
C(5)	2566(1)	6543(1)	3125(2)	17(1)
O(6)	2268(1)	2212(1)	2195(1)	20(1)
C(6)	1937(1)	6454(2)	1730(2)	19(1)
O(7)	1300(1)	3860(1)	4784(1)	24(1)
C(7)	2294(1)	5516(1)	1105(1)	17(1)
C(8)	3305(1)	4718(1)	1895(1)	14(1)
C(9)	2902(1)	4223(1)	3080(1)	14(1)
C(10)	2468(1)	5300(1)	3825(1)	16(1)
C(11)	1177(2)	4990(2)	4052(2)	20(1)
C(12)	184(1)	4774(2)	2835(2)	21(1)
C(13)	632(1)	3748(2)	2105(1)	18(1)
C(14)	1882(1)	3229(1)	2807(1)	15(1)
C(15)	1668(2)	2828(1)	4114(2)	20(1)

Table 3. Selected bond lengths [Å] and angles [°] for s17sel12.

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for s17sel12.

O(1)-C(1)	1.195(2)
C(1)-O(3)	1.334(2)
C(1)-O(2)	1.3534(18)
O(2)-C(3)	1.4517(17)
C(2)-O(3)	1.446(2)
C(2)-C(3)	1.526(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(8)	1.541(2)
C(3)-C(4)	1.547(2)
O(4)-C(4)	1.2026(19)
C(4)-C(5)	1.520(2)
O(5)-C(13)	1.213(2)
C(5)-C(6)	1.515(2)
C(5)-C(10)	1.561(2)
C(5)-H(5)	1.0000
O(6)-C(14)	1.4007(18)
O(6)-H(1)	0.86(3)
C(6)-C(7)	1.328(2)
C(6)-H(6)	0.9500
O(7)-C(15)	1.4389(19)
O(7)-C(11)	1.4472(19)
C(7)-C(8)	1.512(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.5446(19)
C(8)-H(8)	1.0000
C(9)-C(14)	1.5353(19)
C(9)-C(10)	1.5537(19)
C(9)-H(9)	1.0000
C(10)-C(11)	1.534(2)
C(10)-H(10)	1.0000
C(11)-C(12)	1.526(2)
C(11)-H(11)	1.0000
C(12)-C(13)	1.509(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(13)-C(14)	1.520(2)
C(14)-C(15)	1.547(2)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900

O(1)-C(1)-O(3)	125.56(15)
O(1)-C(1)-O(2)	123.01(15)
O(3)-C(1)-O(2)	111.42(13)
C(1)-O(2)-C(3)	109.20(11)
O(3)-C(2)-C(3)	102.93(12)
O(3)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
O(3)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
C(1)-O(3)-C(2)	108.73(11)
O(2)-C(3)-C(2)	101.62(11)
O(2)-C(3)-C(8)	111.23(11)
C(2)-C(3)-C(8)	114.38(12)
O(2)-C(3)-C(4)	107.47(11)
C(2)-C(3)-C(4)	112.93(12)
C(8)-C(3)-C(4)	108.85(11)
O(4)-C(4)-C(5)	126.56(14)
O(4)-C(4)-C(3)	121.56(13)
C(5)-C(4)-C(3)	111.85(12)
C(6)-C(5)-C(4)	105.11(12)
C(6)-C(5)-C(10)	111.25(12)
C(4)-C(5)-C(10)	103.22(12)
C(6)-C(5)-H(5)	112.2
C(4)-C(5)-H(5)	112.2
C(10)-C(5)-H(5)	112.2
C(14)-O(6)-H(1)	109.4(19)
C(7)-C(6)-C(5)	115.82(14)
C(7)-C(6)-H(6)	122.1
C(5)-C(6)-H(6)	122.1
C(15)-O(7)-C(11)	112.58(11)
C(6)-C(7)-C(8)	114.48(13)
C(6)-C(7)-H(7)	122.8

C(8)-C(7)-H(7)	122.8
C(7)-C(8)-C(3)	104.15(12)
C(7)-C(8)-C(9)	110.76(12)
C(3)-C(8)-C(9)	106.75(11)
C(7)-C(8)-H(8)	111.6
C(3)-C(8)-H(8)	111.6
C(9)-C(8)-H(8)	111.6
C(14)-C(9)-C(8)	114.83(12)
C(14)-C(9)-C(10)	109.13(11)
C(8)-C(9)-C(10)	110.52(12)
C(14)-C(9)-H(9)	107.3
C(8)-C(9)-H(9)	107.3
C(10)-C(9)-H(9)	107.3
C(11)-C(10)-C(9)	108.98(12)
C(11)-C(10)-C(5)	115.79(13)
C(9)-C(10)-C(5)	109.42(11)
C(11)-C(10)-H(10)	107.4
C(9)-C(10)-H(10)	107.4
C(5)-C(10)-H(10)	107.4
O(7)-C(11)-C(12)	107.55(13)
O(7)-C(11)-C(10)	107.28(12)
C(12)-C(11)-C(10)	113.72(13)
O(7)-C(11)-H(11)	109.4
C(12)-C(11)-H(11)	109.4
C(10)-C(11)-H(11)	109.4
C(13)-C(12)-C(11)	108.06(12)
C(13)-C(12)-H(12A)	110.1
C(11)-C(12)-H(12A)	110.1
C(13)-C(12)-H(12B)	110.1
C(11)-C(12)-H(12B)	110.1
H(12A)-C(12)-H(12B)	108.4
O(5)-C(13)-C(12)	125.48(14)
O(5)-C(13)-C(14)	122.13(14)
C(12)-C(13)-C(14)	112.15(13)
O(6)-C(14)-C(13)	113.07(12)
O(6)-C(14)-C(9)	110.77(12)
C(13)-C(14)-C(9)	112.09(12)
O(6)-C(14)-C(15)	109.73(12)

C(13)-C(14)-C(15)	104.60(12)
C(9)-C(14)-C(15)	106.15(12)
O(7)-C(15)-C(14)	111.17(12)
O(7)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15A)	109.4
O(7)-C(15)-H(15B)	109.4
C(14)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17sel12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(1)	27(1)	40(1)	-9(1)	5(1)	3(1)
C(1)	15(1)	18(1)	25(1)	-9(1)	6(1)	-4(1)
O(2)	12(1)	21(1)	17(1)	0(1)	3(1)	2(1)
C(2)	21(1)	19(1)	19(1)	-1(1)	8(1)	-4(1)
O(3)	20(1)	26(1)	22(1)	-7(1)	11(1)	-5(1)
C(3)	14(1)	15(1)	13(1)	0(1)	2(1)	1(1)
O(4)	22(1)	22(1)	28(1)	-9(1)	5(1)	-4(1)
C(4)	18(1)	14(1)	15(1)	1(1)	4(1)	1(1)
O(5)	21(1)	34(1)	26(1)	-4(1)	-2(1)	0(1)
C(5)	16(1)	15(1)	21(1)	-2(1)	6(1)	1(1)
O(6)	20(1)	17(1)	21(1)	-4(1)	3(1)	1(1)
C(6)	15(1)	19(1)	23(1)	6(1)	2(1)	1(1)
O(7)	31(1)	23(1)	21(1)	2(1)	13(1)	0(1)
C(7)	16(1)	20(1)	15(1)	3(1)	1(1)	-4(1)
C(8)	15(1)	15(1)	13(1)	-1(1)	4(1)	-1(1)
C(9)	14(1)	14(1)	13(1)	1(1)	2(1)	0(1)
C(10)	17(1)	17(1)	14(1)	-1(1)	5(1)	0(1)
C(11)	22(1)	20(1)	22(1)	1(1)	10(1)	1(1)
C(12)	14(1)	21(1)	27(1)	2(1)	8(1)	2(1)
C(13)	15(1)	20(1)	20(1)	3(1)	4(1)	-3(1)
C(14)	16(1)	13(1)	16(1)	1(1)	5(1)	0(1)
C(15)	25(1)	17(1)	19(1)	3(1)	7(1)	-1(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for s17sel12.

	x	y	z	U(eq)
H(1)	1670(30)	1990(30)	1570(30)	55(8)
H(2A)	4406	6083	496	23
H(2B)	5262	6993	1515	23
H(5)	2253	7259	3548	21
H(6)	1326	7033	1326	23
H(7)	1942	5360	233	21
H(8)	3551	4033	1382	17
H(9)	3654	3844	3647	16
H(10)	3062	5345	4673	19
H(11)	900	5671	4549	24
H(12A)	-616	4540	3041	25
H(12B)	52	5537	2318	25
H(15A)	1011	2186	3991	24
H(15B)	2446	2465	4627	24

Table 7. Torsion angles [°] for s17sel12.

O(1)-C(1)-O(2)-C(3)	-172.66(14)
O(3)-C(1)-O(2)-C(3)	6.03(16)
O(1)-C(1)-O(3)-C(2)	-170.54(15)
O(2)-C(1)-O(3)-C(2)	10.81(16)
C(3)-C(2)-O(3)-C(1)	-21.88(15)
C(1)-O(2)-C(3)-C(2)	-18.84(14)
C(1)-O(2)-C(3)-C(8)	103.30(13)
C(1)-O(2)-C(3)-C(4)	-137.64(12)
O(3)-C(2)-C(3)-O(2)	23.82(14)
O(3)-C(2)-C(3)-C(8)	-96.13(14)
O(3)-C(2)-C(3)-C(4)	138.64(12)
O(2)-C(3)-C(4)-O(4)	51.78(18)
C(2)-C(3)-C(4)-O(4)	-59.47(19)
C(8)-C(3)-C(4)-O(4)	172.36(14)
O(2)-C(3)-C(4)-C(5)	-126.35(12)
C(2)-C(3)-C(4)-C(5)	122.40(13)
C(8)-C(3)-C(4)-C(5)	-5.77(16)
O(4)-C(4)-C(5)-C(6)	131.00(16)
C(3)-C(4)-C(5)-C(6)	-50.99(15)
O(4)-C(4)-C(5)-C(10)	-112.31(17)
C(3)-C(4)-C(5)-C(10)	65.70(14)
C(4)-C(5)-C(6)-C(7)	58.46(17)
C(10)-C(5)-C(6)-C(7)	-52.58(18)
C(5)-C(6)-C(7)-C(8)	-1.89(19)
C(6)-C(7)-C(8)-C(3)	-58.58(16)
C(6)-C(7)-C(8)-C(9)	55.84(17)
O(2)-C(3)-C(8)-C(7)	178.06(11)
C(2)-C(3)-C(8)-C(7)	-67.53(15)
C(4)-C(3)-C(8)-C(7)	59.83(14)
O(2)-C(3)-C(8)-C(9)	60.83(14)
C(2)-C(3)-C(8)-C(9)	175.24(12)
C(4)-C(3)-C(8)-C(9)	-57.40(14)
C(7)-C(8)-C(9)-C(14)	71.54(16)
C(3)-C(8)-C(9)-C(14)	-175.69(12)
C(7)-C(8)-C(9)-C(10)	-52.44(15)
C(3)-C(8)-C(9)-C(10)	60.33(14)

C(14)-C(9)-C(10)-C(11)	0.91(16)
C(8)-C(9)-C(10)-C(11)	128.11(13)
C(14)-C(9)-C(10)-C(5)	-126.61(13)
C(8)-C(9)-C(10)-C(5)	0.58(16)
C(6)-C(5)-C(10)-C(11)	-73.28(16)
C(4)-C(5)-C(10)-C(11)	174.47(12)
C(6)-C(5)-C(10)-C(9)	50.32(16)
C(4)-C(5)-C(10)-C(9)	-61.93(14)
C(15)-O(7)-C(11)-C(12)	59.88(16)
C(15)-O(7)-C(11)-C(10)	-62.82(16)
C(9)-C(10)-C(11)-O(7)	60.13(15)
C(5)-C(10)-C(11)-O(7)	-176.04(12)
C(9)-C(10)-C(11)-C(12)	-58.66(16)
C(5)-C(10)-C(11)-C(12)	65.17(17)
O(7)-C(11)-C(12)-C(13)	-61.57(15)
C(10)-C(11)-C(12)-C(13)	57.08(17)
C(11)-C(12)-C(13)-O(5)	176.32(15)
C(11)-C(12)-C(13)-C(14)	1.83(17)
O(5)-C(13)-C(14)-O(6)	0.6(2)
C(12)-C(13)-C(14)-O(6)	175.27(12)
O(5)-C(13)-C(14)-C(9)	126.64(15)
C(12)-C(13)-C(14)-C(9)	-58.66(16)
O(5)-C(13)-C(14)-C(15)	-118.79(16)
C(12)-C(13)-C(14)-C(15)	55.92(15)
C(8)-C(9)-C(14)-O(6)	58.44(16)
C(10)-C(9)-C(14)-O(6)	-176.85(11)
C(8)-C(9)-C(14)-C(13)	-68.88(16)
C(10)-C(9)-C(14)-C(13)	55.84(15)
C(8)-C(9)-C(14)-C(15)	177.50(12)
C(10)-C(9)-C(14)-C(15)	-57.79(15)
C(11)-O(7)-C(15)-C(14)	2.25(17)
O(6)-C(14)-C(15)-O(7)	178.54(12)
C(13)-C(14)-C(15)-O(7)	-59.88(15)
C(9)-C(14)-C(15)-O(7)	58.81(16)

Symmetry transformations used to generate equivalent atoms:

Table 8. Hydrogen bonds for s17sel12 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(1)...O(5)	0.86(3)	2.25(3)	2.7264(17)	115(2)

Symmetry transformations used to generate equivalent atoms:

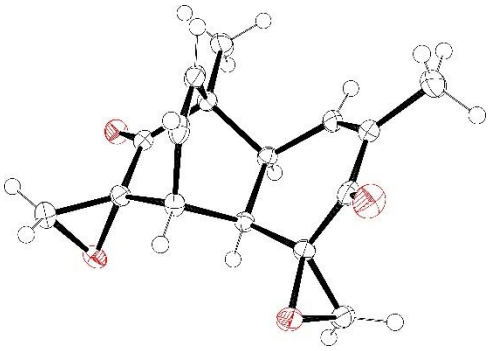


Table 1. Crystal data and structure refinement for s17sel10.

Identification code	s17sel10	
Empirical formula	C16 H16 O4	
Formula weight	272.29	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0979(4) Å	α= 69.194(4)°.
	b = 8.9056(4) Å	β= 70.888(4)°.
	c = 10.6159(5) Å	γ = 68.673(4)°.
Volume	649.15(6) $Å^3$	
Z	2	
Density (calculated)	1.393 Mg/m^3	
Absorption coefficient	0.821 mm^{-1}	
F(000)	288	
Crystal size	0.320 x 0.220 x 0.100 mm^3	
Theta range for data collection	4.576 to 72.780°.	
Index ranges	-9<=h<=9, -6<=k<=11, -11<=l<=13	
Reflections collected	4609	
Independent reflections	2555 [R(int) = 0.0143]	
Completeness to theta = 67.684°	99.9 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.80340
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2555 / 0 / 183
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0975
R indices (all data)	R1 = 0.0393, wR2 = 0.0996
Extinction coefficient	n/a
Largest diff. peak and hole	0.313 and -0.220 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17sel10. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3162(2)	-184(2)	2984(1)	20(1)
C(2)	1543(2)	935(2)	2440(1)	22(1)
C(3)	-22(2)	228(2)	2781(2)	38(1)
C(4)	1543(2)	2494(2)	1677(1)	21(1)
C(5)	2944(2)	3354(1)	1448(1)	16(1)
C(6)	4689(2)	2182(1)	1962(1)	16(1)
C(7)	4861(2)	357(2)	2219(1)	17(1)
C(8)	6203(2)	-602(2)	1254(1)	22(1)
C(9)	4734(2)	2556(2)	3276(1)	18(1)
C(10)	5012(2)	4285(2)	2761(1)	17(1)
C(11)	6041(2)	4810(2)	3356(1)	22(1)
C(12)	3502(2)	5543(2)	2073(1)	17(1)
C(13)	2001(2)	4786(2)	2236(1)	18(1)
C(14)	411(2)	6122(2)	1668(2)	28(1)
C(15)	1532(2)	3883(2)	3754(1)	22(1)
C(16)	2900(2)	2728(2)	4276(1)	22(1)
O(1)	3162(1)	-1475(1)	3903(1)	31(1)
O(2)	6517(1)	-790(1)	2572(1)	23(1)
O(3)	6806(1)	4453(1)	2019(1)	22(1)
O(4)	3532(1)	6962(1)	1433(1)	23(1)

Table 3. Bond lengths [Å] for s17sel10.

C(1)-O(1)	1.2157(16)
C(1)-C(2)	1.4766(18)
C(1)-C(7)	1.5026(17)
C(2)-C(4)	1.3365(19)
C(2)-C(3)	1.5004(18)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(5)	1.5004(16)
C(4)-H(4)	0.9500
C(5)-C(6)	1.5525(15)
C(5)-C(13)	1.5937(16)
C(5)-H(5)	1.0000
C(6)-C(7)	1.5105(16)
C(6)-C(9)	1.5590(16)
C(6)-H(6)	1.0000
C(7)-O(2)	1.4291(14)
C(7)-C(8)	1.4752(17)
C(8)-O(2)	1.4444(15)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(16)	1.5076(17)
C(9)-C(10)	1.5148(16)
C(9)-H(9)	1.0000
C(10)-O(3)	1.4420(14)
C(10)-C(11)	1.4670(17)
C(10)-C(12)	1.5134(16)
C(11)-O(3)	1.4503(16)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-O(4)	1.2083(15)
C(12)-C(13)	1.5293(16)
C(13)-C(15)	1.5133(18)
C(13)-C(14)	1.5237(17)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800

C(14)-H(14C)	0.9800
C(15)-C(16)	1.3263(19)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500

Table 4. Bond angles [°] for s17sel10.

O(1)-C(1)-C(2)	123.80(12)
O(1)-C(1)-C(7)	122.57(12)
C(2)-C(1)-C(7)	113.49(10)
C(4)-C(2)-C(1)	119.29(11)
C(4)-C(2)-C(3)	123.65(13)
C(1)-C(2)-C(3)	117.06(12)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-C(5)	126.49(11)
C(2)-C(4)-H(4)	116.8
C(5)-C(4)-H(4)	116.8
C(4)-C(5)-C(6)	114.40(10)
C(4)-C(5)-C(13)	107.25(9)
C(6)-C(5)-C(13)	109.39(9)
C(4)-C(5)-H(5)	108.6
C(6)-C(5)-H(5)	108.6
C(13)-C(5)-H(5)	108.6
C(7)-C(6)-C(5)	112.31(9)
C(7)-C(6)-C(9)	111.55(9)
C(5)-C(6)-C(9)	109.84(9)
C(7)-C(6)-H(6)	107.6
C(5)-C(6)-H(6)	107.6
C(9)-C(6)-H(6)	107.6
O(2)-C(7)-C(8)	59.62(8)
O(2)-C(7)-C(1)	116.10(10)
C(8)-C(7)-C(1)	116.79(10)
O(2)-C(7)-C(6)	115.42(10)
C(8)-C(7)-C(6)	120.57(11)
C(1)-C(7)-C(6)	116.14(10)
O(2)-C(8)-C(7)	58.60(7)
O(2)-C(8)-H(8A)	117.9
C(7)-C(8)-H(8A)	117.9

O(2)-C(8)-H(8B)	117.9
C(7)-C(8)-H(8B)	117.9
H(8A)-C(8)-H(8B)	115.1
C(16)-C(9)-C(10)	105.27(10)
C(16)-C(9)-C(6)	110.84(10)
C(10)-C(9)-C(6)	104.74(9)
C(16)-C(9)-H(9)	111.9
C(10)-C(9)-H(9)	111.9
C(6)-C(9)-H(9)	111.9
O(3)-C(10)-C(11)	59.80(8)
O(3)-C(10)-C(12)	114.11(10)
C(11)-C(10)-C(12)	121.09(10)
O(3)-C(10)-C(9)	118.29(10)
C(11)-C(10)-C(9)	123.32(10)
C(12)-C(10)-C(9)	110.56(10)
O(3)-C(11)-C(10)	59.25(7)
O(3)-C(11)-H(11A)	117.8
C(10)-C(11)-H(11A)	117.8
O(3)-C(11)-H(11B)	117.8
C(10)-C(11)-H(11B)	117.8
H(11A)-C(11)-H(11B)	115.0
O(4)-C(12)-C(10)	123.15(11)
O(4)-C(12)-C(13)	124.64(11)
C(10)-C(12)-C(13)	112.17(10)
C(15)-C(13)-C(14)	115.14(11)
C(15)-C(13)-C(12)	105.87(10)
C(14)-C(13)-C(12)	110.97(10)
C(15)-C(13)-C(5)	105.48(9)
C(14)-C(13)-C(5)	112.92(10)
C(12)-C(13)-C(5)	105.76(9)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-C(13)	116.18(11)
C(16)-C(15)-H(15)	121.9

C(13)-C(15)-H(15)	121.9
C(15)-C(16)-C(9)	114.84(11)
C(15)-C(16)-H(16)	122.6
C(9)-C(16)-H(16)	122.6
C(7)-O(2)-C(8)	61.77(7)
C(10)-O(3)-C(11)	60.95(8)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17sel10. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(1)	16(1)	21(1)	-8(1)	-2(1)	-7(1)
C(2)	18(1)	23(1)	30(1)	-14(1)	-2(1)	-6(1)
C(3)	24(1)	30(1)	69(1)	-22(1)	-6(1)	-10(1)
C(4)	18(1)	22(1)	27(1)	-12(1)	-9(1)	-2(1)
C(5)	18(1)	14(1)	17(1)	-4(1)	-6(1)	-2(1)
C(6)	15(1)	15(1)	16(1)	-4(1)	-4(1)	-4(1)
C(7)	17(1)	15(1)	18(1)	-3(1)	-8(1)	-2(1)
C(8)	21(1)	20(1)	24(1)	-8(1)	-6(1)	-2(1)
C(9)	21(1)	15(1)	18(1)	-3(1)	-8(1)	-5(1)
C(10)	17(1)	17(1)	17(1)	-4(1)	-4(1)	-6(1)
C(11)	25(1)	22(1)	23(1)	-5(1)	-9(1)	-9(1)
C(12)	18(1)	16(1)	17(1)	-6(1)	-3(1)	-4(1)
C(13)	16(1)	15(1)	24(1)	-7(1)	-5(1)	-3(1)
C(14)	21(1)	19(1)	47(1)	-12(1)	-15(1)	0(1)
C(15)	22(1)	25(1)	22(1)	-13(1)	2(1)	-11(1)
C(16)	30(1)	23(1)	15(1)	-5(1)	-2(1)	-14(1)
O(1)	38(1)	21(1)	28(1)	-1(1)	-4(1)	-12(1)
O(2)	21(1)	19(1)	28(1)	-7(1)	-13(1)	2(1)
O(3)	17(1)	26(1)	24(1)	-6(1)	-4(1)	-8(1)
O(4)	26(1)	16(1)	27(1)	-2(1)	-8(1)	-7(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17sel10.

	x	y	z	U(eq)
H(3A)	-944	1032	2273	58
H(3B)	-559	13	3777	58
H(3C)	414	-821	2514	58
H(4)	558	3121	1236	25
H(5)	3302	3890	435	20
H(6)	5761	2446	1218	19
H(8A)	5905	-1527	1145	26
H(8B)	6922	6	408	26
H(9)	5726	1701	3725	21
H(11A)	5640	5994	3376	26
H(11B)	6550	3996	4150	26
H(14A)	-110	6971	2183	42
H(14B)	-522	5604	1767	42
H(14C)	842	6649	687	42
H(15)	327	4128	4303	26
H(16)	2737	2061	5207	26

Table 7. Torsion angles [°] for s17sel10.

O(1)-C(1)-C(2)-C(4)	164.24(13)
C(7)-C(1)-C(2)-C(4)	-20.07(16)
O(1)-C(1)-C(2)-C(3)	-16.09(19)
C(7)-C(1)-C(2)-C(3)	159.61(12)
C(1)-C(2)-C(4)-C(5)	-8.82(19)
C(3)-C(2)-C(4)-C(5)	171.52(13)
C(2)-C(4)-C(5)-C(6)	10.69(18)
C(2)-C(4)-C(5)-C(13)	-110.81(14)
C(4)-C(5)-C(6)-C(7)	16.06(14)
C(13)-C(5)-C(6)-C(7)	136.39(10)
C(4)-C(5)-C(6)-C(9)	-108.70(11)
C(13)-C(5)-C(6)-C(9)	11.63(12)
O(1)-C(1)-C(7)-O(2)	3.88(17)
C(2)-C(1)-C(7)-O(2)	-171.88(10)
O(1)-C(1)-C(7)-C(8)	71.33(16)
C(2)-C(1)-C(7)-C(8)	-104.43(12)
O(1)-C(1)-C(7)-C(6)	-136.73(12)
C(2)-C(1)-C(7)-C(6)	47.51(14)
C(5)-C(6)-C(7)-O(2)	174.51(9)
C(9)-C(6)-C(7)-O(2)	-61.69(13)
C(5)-C(6)-C(7)-C(8)	106.20(12)
C(9)-C(6)-C(7)-C(8)	-130.00(11)
C(5)-C(6)-C(7)-C(1)	-44.61(14)
C(9)-C(6)-C(7)-C(1)	79.19(13)
C(1)-C(7)-C(8)-O(2)	-105.98(11)
C(6)-C(7)-C(8)-O(2)	103.39(12)
C(7)-C(6)-C(9)-C(16)	-80.29(12)
C(5)-C(6)-C(9)-C(16)	44.90(13)
C(7)-C(6)-C(9)-C(10)	166.66(10)
C(5)-C(6)-C(9)-C(10)	-68.15(11)
C(16)-C(9)-C(10)-O(3)	166.80(10)
C(6)-C(9)-C(10)-O(3)	-76.26(12)
C(16)-C(9)-C(10)-C(11)	96.06(13)
C(6)-C(9)-C(10)-C(11)	-147.00(11)
C(16)-C(9)-C(10)-C(12)	-58.98(12)
C(6)-C(9)-C(10)-C(12)	57.96(12)

C(12)-C(10)-C(11)-O(3)	-101.60(12)
C(9)-C(10)-C(11)-O(3)	105.88(12)
O(3)-C(10)-C(12)-O(4)	-34.47(16)
C(11)-C(10)-C(12)-O(4)	33.59(17)
C(9)-C(10)-C(12)-O(4)	-170.73(11)
O(3)-C(10)-C(12)-C(13)	143.18(10)
C(11)-C(10)-C(12)-C(13)	-148.76(11)
C(9)-C(10)-C(12)-C(13)	6.92(13)
O(4)-C(12)-C(13)-C(15)	-133.93(12)
C(10)-C(12)-C(13)-C(15)	48.46(12)
O(4)-C(12)-C(13)-C(14)	-8.34(17)
C(10)-C(12)-C(13)-C(14)	174.05(10)
O(4)-C(12)-C(13)-C(5)	114.45(13)
C(10)-C(12)-C(13)-C(5)	-63.16(12)
C(4)-C(5)-C(13)-C(15)	63.91(12)
C(6)-C(5)-C(13)-C(15)	-60.70(12)
C(4)-C(5)-C(13)-C(14)	-62.65(13)
C(6)-C(5)-C(13)-C(14)	172.74(10)
C(4)-C(5)-C(13)-C(12)	175.80(10)
C(6)-C(5)-C(13)-C(12)	51.20(12)
C(14)-C(13)-C(15)-C(16)	-179.24(11)
C(12)-C(13)-C(15)-C(16)	-56.25(13)
C(5)-C(13)-C(15)-C(16)	55.57(13)
C(13)-C(15)-C(16)-C(9)	2.63(16)
C(10)-C(9)-C(16)-C(15)	56.23(13)
C(6)-C(9)-C(16)-C(15)	-56.48(14)
C(1)-C(7)-O(2)-C(8)	107.13(12)
C(6)-C(7)-O(2)-C(8)	-111.97(12)
C(12)-C(10)-O(3)-C(11)	113.21(11)
C(9)-C(10)-O(3)-C(11)	-114.12(12)

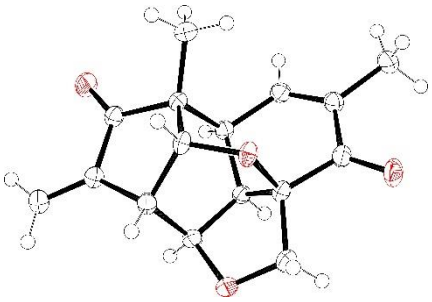


Table 1. Crystal data and structure refinement for s17sel9.

Identification code	s17sel9	
Empirical formula	C16 H16 O4	
Formula weight	272.29	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 5.78650(10) Å	α= 90°.
	b = 14.3271(2) Å	β= 100.616(2)°.
	c = 15.5733(3) Å	γ = 90°.
Volume	1268.99(4) $Å^3$	
Z	4	
Density (calculated)	1.425 Mg/m^3	
Absorption coefficient	0.840 mm^{-1}	
F(000)	576	
Crystal size	0.280 x 0.200 x 0.100 mm^3	
Theta range for data collection	4.227 to 72.995°.	
Index ranges	-7<=h<=6, -11<=k<=17, -19<=l<=17	
Reflections collected	10355	
Independent reflections	2520 [R(int) = 0.0245]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.89349	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2520 / 0 / 183	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0901	
R indices (all data)	R1 = 0.0392, wR2 = 0.0919	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.286 and -0.211 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17sel9. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-330(2)	2804(1)	2972(1)	21(1)
C(2)	425(2)	3791(1)	3096(1)	23(1)
C(3)	-1163(3)	4512(1)	2595(1)	29(1)
C(4)	2437(2)	4000(1)	3641(1)	22(1)
C(5)	4067(2)	3306(1)	4180(1)	18(1)
C(6)	3735(2)	2347(1)	3736(1)	18(1)
C(7)	1116(2)	2118(1)	3588(1)	19(1)
C(8)	1070(2)	1105(1)	3312(1)	25(1)
C(9)	4627(2)	1469(1)	4252(1)	21(1)
C(10)	4072(2)	1553(1)	5182(1)	20(1)
C(11)	2149(2)	2301(1)	5149(1)	19(1)
C(12)	3520(2)	3224(1)	5135(1)	19(1)
C(13)	2304(2)	4069(1)	5441(1)	28(1)
C(14)	5828(2)	3008(1)	5754(1)	21(1)
C(15)	6115(2)	1975(1)	5801(1)	20(1)
C(16)	7853(2)	1546(1)	6330(1)	24(1)
O(1)	-2009(2)	2555(1)	2428(1)	30(1)
O(2)	283(1)	2210(1)	4406(1)	21(1)
O(3)	3260(2)	730(1)	3778(1)	27(1)
O(4)	7158(2)	3582(1)	6144(1)	30(1)

Table 3. Bond lengths [Å] for s17sel9.

C(1)-O(1)	1.2184(16)
C(1)-C(2)	1.4823(18)
C(1)-C(7)	1.5134(17)
C(2)-C(4)	1.3421(18)
C(2)-C(3)	1.5016(17)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(5)	1.5130(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.5344(16)
C(5)-C(12)	1.5820(16)
C(5)-H(5)	1.0000
C(6)-C(7)	1.5258(16)
C(6)-C(9)	1.5298(16)
C(6)-H(6)	1.0000
C(7)-O(2)	1.4494(14)
C(7)-C(8)	1.5120(17)
C(8)-O(3)	1.4431(15)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-O(3)	1.4411(14)
C(9)-C(10)	1.5456(17)
C(9)-H(9)	1.0000
C(10)-C(15)	1.5072(16)
C(10)-C(11)	1.5394(17)
C(10)-H(10)	1.0000
C(11)-O(2)	1.4356(14)
C(11)-C(12)	1.5435(16)
C(11)-H(11)	1.0000
C(12)-C(13)	1.5202(17)
C(12)-C(14)	1.5274(16)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-O(4)	1.2109(16)

C(14)-C(15)	1.4895(17)
C(15)-C(16)	1.3272(18)
C(16)-H(16A)	0.9500
C(16)-H(16B)	0.9500

Table 4. Bond angles [°] for s17sel9.

O(1)-C(1)-C(2)	123.27(12)
O(1)-C(1)-C(7)	121.81(12)
C(2)-C(1)-C(7)	114.90(10)
C(4)-C(2)-C(1)	119.75(11)
C(4)-C(2)-C(3)	123.48(12)
C(1)-C(2)-C(3)	116.76(11)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-C(5)	125.69(11)
C(2)-C(4)-H(4)	117.2
C(5)-C(4)-H(4)	117.2
C(4)-C(5)-C(6)	109.01(10)
C(4)-C(5)-C(12)	111.00(10)
C(6)-C(5)-C(12)	109.00(9)
C(4)-C(5)-H(5)	109.3
C(6)-C(5)-H(5)	109.3
C(12)-C(5)-H(5)	109.3
C(7)-C(6)-C(9)	97.64(9)
C(7)-C(6)-C(5)	107.41(9)
C(9)-C(6)-C(5)	119.89(10)
C(7)-C(6)-H(6)	110.3
C(9)-C(6)-H(6)	110.3
C(5)-C(6)-H(6)	110.3
O(2)-C(7)-C(8)	110.16(10)
O(2)-C(7)-C(1)	105.32(9)
C(8)-C(7)-C(1)	117.69(10)
O(2)-C(7)-C(6)	109.21(9)
C(8)-C(7)-C(6)	102.36(10)
C(1)-C(7)-C(6)	112.01(10)
O(3)-C(8)-C(7)	104.32(9)
O(3)-C(8)-H(8A)	110.9
C(7)-C(8)-H(8A)	110.9

O(3)-C(8)-H(8B)	110.9
C(7)-C(8)-H(8B)	110.9
H(8A)-C(8)-H(8B)	108.9
O(3)-C(9)-C(6)	103.59(9)
O(3)-C(9)-C(10)	110.34(10)
C(6)-C(9)-C(10)	108.66(10)
O(3)-C(9)-H(9)	111.3
C(6)-C(9)-H(9)	111.3
C(10)-C(9)-H(9)	111.3
C(15)-C(10)-C(11)	102.67(10)
C(15)-C(10)-C(9)	110.88(10)
C(11)-C(10)-C(9)	107.21(9)
C(15)-C(10)-H(10)	111.9
C(11)-C(10)-H(10)	111.9
C(9)-C(10)-H(10)	111.9
O(2)-C(11)-C(10)	113.29(10)
O(2)-C(11)-C(12)	112.30(10)
C(10)-C(11)-C(12)	103.11(9)
O(2)-C(11)-H(11)	109.3
C(10)-C(11)-H(11)	109.3
C(12)-C(11)-H(11)	109.3
C(13)-C(12)-C(14)	111.44(10)
C(13)-C(12)-C(11)	114.13(11)
C(14)-C(12)-C(11)	102.11(9)
C(13)-C(12)-C(5)	114.77(10)
C(14)-C(12)-C(5)	107.77(10)
C(11)-C(12)-C(5)	105.64(9)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(4)-C(14)-C(15)	126.55(12)
O(4)-C(14)-C(12)	125.43(12)
C(15)-C(14)-C(12)	108.01(10)
C(16)-C(15)-C(14)	123.75(11)
C(16)-C(15)-C(10)	128.78(12)

C(14)-C(15)-C(10)	107.43(10)
C(15)-C(16)-H(16A)	120.0
C(15)-C(16)-H(16B)	120.0
H(16A)-C(16)-H(16B)	120.0
C(11)-O(2)-C(7)	113.22(9)
C(9)-O(3)-C(8)	109.38(9)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17sel9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	27(1)	18(1)	-1(1)	3(1)	1(1)
C(2)	26(1)	23(1)	19(1)	2(1)	4(1)	4(1)
C(3)	34(1)	29(1)	24(1)	3(1)	2(1)	10(1)
C(4)	28(1)	17(1)	22(1)	1(1)	4(1)	-1(1)
C(5)	18(1)	17(1)	20(1)	-1(1)	2(1)	-3(1)
C(6)	17(1)	18(1)	18(1)	-1(1)	3(1)	0(1)
C(7)	19(1)	21(1)	17(1)	-2(1)	1(1)	-3(1)
C(8)	26(1)	22(1)	25(1)	-3(1)	-4(1)	-3(1)
C(9)	21(1)	17(1)	22(1)	-3(1)	1(1)	0(1)
C(10)	22(1)	18(1)	20(1)	2(1)	0(1)	-3(1)
C(11)	18(1)	24(1)	16(1)	0(1)	1(1)	-4(1)
C(12)	20(1)	18(1)	18(1)	-2(1)	1(1)	-1(1)
C(13)	31(1)	26(1)	25(1)	-6(1)	3(1)	6(1)
C(14)	21(1)	22(1)	19(1)	-1(1)	2(1)	-3(1)
C(15)	20(1)	21(1)	19(1)	1(1)	3(1)	-2(1)
C(16)	22(1)	25(1)	22(1)	3(1)	2(1)	-2(1)
O(1)	22(1)	36(1)	26(1)	0(1)	-6(1)	-1(1)
O(2)	15(1)	29(1)	17(1)	0(1)	1(1)	-4(1)
O(3)	31(1)	18(1)	29(1)	-6(1)	-5(1)	0(1)
O(4)	30(1)	25(1)	31(1)	-4(1)	-7(1)	-6(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17sel9.

	x	y	z	U(eq)
H(3A)	-472	5133	2719	44
H(3B)	-2703	4489	2771	44
H(3C)	-1351	4383	1968	44
H(4)	2876	4639	3693	27
H(5)	5731	3514	4214	22
H(6)	4300	2360	3167	21
H(8A)	-287	776	3478	30
H(8B)	975	1050	2673	30
H(9)	6347	1374	4269	25
H(10)	3580	941	5401	24
H(11)	1480	2270	5696	23
H(13A)	2151	3982	6052	41
H(13B)	739	4139	5078	41
H(13C)	3237	4630	5389	41
H(16A)	9004	1901	6706	28
H(16B)	7946	884	6332	28

Table 7. Torsion angles [°] for s17sel9.

O(1)-C(1)-C(2)-C(4)	-172.77(12)
C(7)-C(1)-C(2)-C(4)	8.47(17)
O(1)-C(1)-C(2)-C(3)	7.64(18)
C(7)-C(1)-C(2)-C(3)	-171.12(11)
C(1)-C(2)-C(4)-C(5)	-1.31(19)
C(3)-C(2)-C(4)-C(5)	178.25(12)
C(2)-C(4)-C(5)-C(6)	24.90(17)
C(2)-C(4)-C(5)-C(12)	-95.18(14)
C(4)-C(5)-C(6)-C(7)	-53.16(12)
C(12)-C(5)-C(6)-C(7)	68.14(12)
C(4)-C(5)-C(6)-C(9)	-163.10(10)
C(12)-C(5)-C(6)-C(9)	-41.80(14)
O(1)-C(1)-C(7)-O(2)	-100.29(13)
C(2)-C(1)-C(7)-O(2)	78.49(12)
O(1)-C(1)-C(7)-C(8)	22.89(18)
C(2)-C(1)-C(7)-C(8)	-158.33(11)
O(1)-C(1)-C(7)-C(6)	141.11(12)
C(2)-C(1)-C(7)-C(6)	-40.11(14)
C(9)-C(6)-C(7)-O(2)	71.54(11)
C(5)-C(6)-C(7)-O(2)	-53.15(12)
C(9)-C(6)-C(7)-C(8)	-45.20(11)
C(5)-C(6)-C(7)-C(8)	-169.89(9)
C(9)-C(6)-C(7)-C(1)	-172.19(10)
C(5)-C(6)-C(7)-C(1)	63.12(12)
O(2)-C(7)-C(8)-O(3)	-84.30(12)
C(1)-C(7)-C(8)-O(3)	155.00(10)
C(6)-C(7)-C(8)-O(3)	31.76(12)
C(7)-C(6)-C(9)-O(3)	43.13(11)
C(5)-C(6)-C(9)-O(3)	158.30(10)
C(7)-C(6)-C(9)-C(10)	-74.20(11)
C(5)-C(6)-C(9)-C(10)	40.97(14)
O(3)-C(9)-C(10)-C(15)	154.41(10)
C(6)-C(9)-C(10)-C(15)	-92.65(12)
O(3)-C(9)-C(10)-C(11)	-94.25(11)
C(6)-C(9)-C(10)-C(11)	18.69(12)
C(15)-C(10)-C(11)-O(2)	161.53(9)

C(9)-C(10)-C(11)-O(2)	44.66(13)
C(15)-C(10)-C(11)-C(12)	39.90(11)
C(9)-C(10)-C(11)-C(12)	-76.97(11)
O(2)-C(11)-C(12)-C(13)	79.56(13)
C(10)-C(11)-C(12)-C(13)	-158.15(10)
O(2)-C(11)-C(12)-C(14)	-160.06(9)
C(10)-C(11)-C(12)-C(14)	-37.77(11)
O(2)-C(11)-C(12)-C(5)	-47.47(12)
C(10)-C(11)-C(12)-C(5)	74.83(11)
C(4)-C(5)-C(12)-C(13)	-23.53(14)
C(6)-C(5)-C(12)-C(13)	-143.61(11)
C(4)-C(5)-C(12)-C(14)	-148.32(10)
C(6)-C(5)-C(12)-C(14)	91.60(11)
C(4)-C(5)-C(12)-C(11)	103.11(11)
C(6)-C(5)-C(12)-C(11)	-16.97(12)
C(13)-C(12)-C(14)-O(4)	-34.88(18)
C(11)-C(12)-C(14)-O(4)	-157.12(12)
C(5)-C(12)-C(14)-O(4)	91.88(14)
C(13)-C(12)-C(14)-C(15)	144.06(11)
C(11)-C(12)-C(14)-C(15)	21.82(12)
C(5)-C(12)-C(14)-C(15)	-89.18(11)
O(4)-C(14)-C(15)-C(16)	3.9(2)
C(12)-C(14)-C(15)-C(16)	-174.98(12)
O(4)-C(14)-C(15)-C(10)	-178.19(12)
C(12)-C(14)-C(15)-C(10)	2.89(13)
C(11)-C(10)-C(15)-C(16)	151.21(13)
C(9)-C(10)-C(15)-C(16)	-94.57(15)
C(11)-C(10)-C(15)-C(14)	-26.52(12)
C(9)-C(10)-C(15)-C(14)	87.71(12)
C(10)-C(11)-O(2)-C(7)	-49.86(13)
C(12)-C(11)-O(2)-C(7)	66.46(13)
C(8)-C(7)-O(2)-C(11)	100.13(11)
C(1)-C(7)-O(2)-C(11)	-132.01(10)
C(6)-C(7)-O(2)-C(11)	-11.55(13)
C(6)-C(9)-O(3)-C(8)	-25.35(13)
C(10)-C(9)-O(3)-C(8)	90.79(12)
C(7)-C(8)-O(3)-C(9)	-3.99(13)

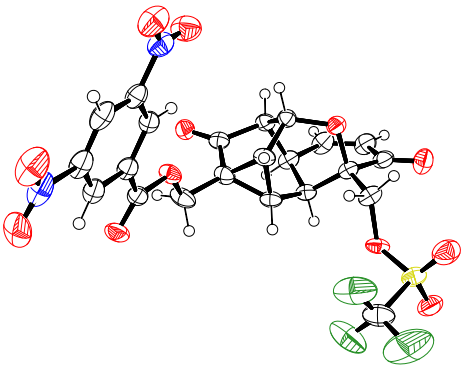


Table 1. Crystal data and structure refinement for s17sel4.

Identification code	s17sel4	
Empirical formula	C22 H15 F3 N2 O12 S	
Formula weight	588.42	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 18.3704(16) Å	α= 90°.
	b = 6.0258(5) Å	β= 93.673(8)°.
	c = 20.643(2) Å	γ = 90°.
Volume	2280.4(4) $Å^3$	
Z	4	
Density (calculated)	1.714 Mg/m^3	
Absorption coefficient	2.183 mm^{-1}	
F(000)	1200	
Crystal size	0.100 x 0.080 x 0.020 mm^3	
Theta range for data collection	3.123 to 73.684°.	
Index ranges	-22<=h<=21, -7<=k<=7, -25<=l<=24	
Reflections collected	13705	
Independent reflections	4511 [R(int) = 0.0697]	
Completeness to theta = 67.684°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.39209	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4511 / 73 / 425	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0781, wR2 = 0.1882	
R indices (all data)	R1 = 0.1285, wR2 = 0.2185	
Extinction coefficient	n/a	

Largest diff. peak and hole	0.613 and -0.636 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17sel4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	1891(2)	6194(11)	8856(2)	56(1)
N(2)	560(2)	520(8)	7523(2)	44(1)
O(1)	1340(2)	6224(5)	5950(1)	35(1)
O(2)	1856(2)	9014(7)	6530(2)	47(1)
O(3)	2152(2)	8066(9)	8878(2)	68(1)
O(4)	1847(2)	4944(10)	9323(2)	72(2)
O(5)	537(2)	-608(7)	8015(2)	57(1)
O(6)	289(2)	19(7)	6991(2)	56(1)
O(7)	102(2)	7183(5)	4491(2)	38(1)
O(8)	2260(2)	-696(7)	2804(2)	53(1)
O(9)	1419(2)	621(5)	3998(2)	33(1)
C(1)	1580(2)	7191(8)	6497(2)	34(1)
C(2)	1455(2)	5784(9)	7074(2)	35(1)
C(3)	1735(2)	6565(9)	7675(2)	39(1)
C(4)	1609(3)	5314(10)	8217(2)	44(1)
C(5)	1235(3)	3340(10)	8188(2)	42(1)
C(6)	966(2)	2651(9)	7582(2)	37(1)
C(7)	1069(2)	3805(8)	7019(2)	32(1)
C(8)	1465(3)	7411(8)	5350(2)	43(1)
C(9)	1317(3)	5863(8)	4793(2)	34(1)
C(10)	597(2)	5897(7)	4423(2)	31(1)
C(11)	608(2)	3958(8)	3961(2)	31(1)
C(12)	998(2)	2138(7)	4376(2)	30(1)
C(13)	1517(2)	3404(8)	4842(2)	32(1)
C(14)	1953(2)	4895(8)	4439(2)	32(1)
C(15)	1891(2)	4259(8)	3720(2)	31(1)
C(16)	1121(2)	4717(8)	3433(2)	34(1)
C(17)	949(3)	3602(10)	2794(2)	42(1)
C(18)	1322(3)	1884(10)	2576(2)	43(1)
C(19)	1903(2)	858(9)	2979(2)	38(1)
C(20)	1999(2)	1727(8)	3677(2)	31(1)
C(21)	2704(2)	876(9)	4015(2)	40(1)
S(1)	4084(1)	1345(4)	3769(1)	42(1)

O(10)	3330(4)	2262(11)	3739(4)	36(2)
O(11)	4109(3)	-946(10)	3932(3)	61(2)
O(12)	4434(4)	2199(14)	3220(4)	53(2)
C(22)	4498(4)	2826(14)	4451(4)	59(2)
F(1)	4477(5)	4948(11)	4357(3)	97(2)
F(2)	4162(4)	2366(14)	4990(3)	97(3)
S(1A)	3957(6)	2480(20)	3905(6)	102(3)
O(10A)	3271(10)	1490(40)	3639(11)	51(6)
O(11A)	3760(20)	4190(50)	4371(17)	182(14)
O(12A)	4370(20)	3010(60)	3345(14)	123(13)
C(22A)	4618(12)	720(30)	4338(15)	148(18)
F(1A)	4733(15)	-900(40)	3907(12)	143(9)
F(2A)	4149(15)	-540(50)	4655(15)	174(12)
F(3)	5179(3)	2122(14)	4545(3)	139(3)

Table 3. Bond lengths [Å] for s17sel4.

N(1)-O(3)	1.225(7)
N(1)-O(4)	1.231(7)
N(1)-C(4)	1.484(6)
N(2)-O(6)	1.215(6)
N(2)-O(5)	1.226(6)
N(2)-C(6)	1.486(7)
O(1)-C(1)	1.322(5)
O(1)-C(8)	1.460(6)
O(2)-C(1)	1.210(6)
O(7)-C(10)	1.209(6)
O(8)-C(19)	1.212(6)
O(9)-C(20)	1.452(5)
O(9)-C(12)	1.456(5)
C(1)-C(2)	1.491(7)
C(2)-C(7)	1.389(7)
C(2)-C(3)	1.394(6)
C(3)-C(4)	1.381(8)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(8)
C(5)-C(6)	1.378(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.378(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.492(6)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.484(6)
C(9)-C(13)	1.528(7)
C(9)-C(14)	1.534(6)
C(10)-C(11)	1.509(6)
C(11)-C(12)	1.539(6)
C(11)-C(16)	1.554(6)
C(11)-H(11)	1.0000
C(12)-C(13)	1.517(6)
C(12)-H(12)	1.0000
C(13)-C(14)	1.492(6)

C(13)-H(13)	1.0000
C(14)-C(15)	1.531(6)
C(14)-H(14)	1.0000
C(15)-C(16)	1.523(6)
C(15)-C(20)	1.542(6)
C(15)-H(15)	1.0000
C(16)-C(17)	1.496(6)
C(16)-H(16)	1.0000
C(17)-C(18)	1.335(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.450(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.533(6)
C(20)-C(21)	1.520(6)
C(21)-O(10A)	1.39(2)
C(21)-O(10)	1.558(9)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(21)-H(21C)	0.9900
C(21)-H(21D)	0.9900
S(1)-O(11)	1.421(6)
S(1)-O(12)	1.434(7)
S(1)-O(10)	1.489(7)
S(1)-C(22)	1.793(8)
C(22)-F(1)	1.293(9)
C(22)-F(3)	1.325(8)
C(22)-F(2)	1.335(9)
S(1A)-O(12A)	1.460(15)
S(1A)-O(10A)	1.469(13)
S(1A)-O(11A)	1.470(15)
S(1A)-C(22A)	1.81(2)
C(22A)-F(1A)	1.347(15)
C(22A)-F(2A)	1.348(15)
C(22A)-F(3)	1.380(15)

Table 4. Bond angles [°] for s17sel4.

O(3)-N(1)-O(4)	125.4(5)
O(3)-N(1)-C(4)	118.4(5)
O(4)-N(1)-C(4)	116.2(6)
O(6)-N(2)-O(5)	125.3(5)
O(6)-N(2)-C(6)	117.7(4)
O(5)-N(2)-C(6)	117.0(5)
C(1)-O(1)-C(8)	116.5(4)
C(20)-O(9)-C(12)	112.8(3)
O(2)-C(1)-O(1)	124.3(5)
O(2)-C(1)-C(2)	123.8(4)
O(1)-C(1)-C(2)	111.8(4)
C(7)-C(2)-C(3)	121.3(5)
C(7)-C(2)-C(1)	121.9(4)
C(3)-C(2)-C(1)	116.9(5)
C(4)-C(3)-C(2)	117.8(5)
C(4)-C(3)-H(3)	121.1
C(2)-C(3)-H(3)	121.1
C(5)-C(4)-C(3)	123.1(4)
C(5)-C(4)-N(1)	119.6(5)
C(3)-C(4)-N(1)	117.3(5)
C(4)-C(5)-C(6)	116.8(5)
C(4)-C(5)-H(5)	121.6
C(6)-C(5)-H(5)	121.6
C(7)-C(6)-C(5)	123.6(5)
C(7)-C(6)-N(2)	117.4(4)
C(5)-C(6)-N(2)	119.0(5)
C(6)-C(7)-C(2)	117.5(4)
C(6)-C(7)-H(7)	121.3
C(2)-C(7)-H(7)	121.3
O(1)-C(8)-C(9)	108.4(4)
O(1)-C(8)-H(8A)	110.0
C(9)-C(8)-H(8A)	110.0
O(1)-C(8)-H(8B)	110.0
C(9)-C(8)-H(8B)	110.0
H(8A)-C(8)-H(8B)	108.4
C(10)-C(9)-C(8)	120.0(4)

C(10)-C(9)-C(13)	104.4(4)
C(8)-C(9)-C(13)	121.6(4)
C(10)-C(9)-C(14)	116.2(4)
C(8)-C(9)-C(14)	119.9(4)
C(13)-C(9)-C(14)	58.3(3)
O(7)-C(10)-C(9)	126.9(4)
O(7)-C(10)-C(11)	127.6(4)
C(9)-C(10)-C(11)	105.5(4)
C(10)-C(11)-C(12)	103.0(3)
C(10)-C(11)-C(16)	104.3(4)
C(12)-C(11)-C(16)	108.6(4)
C(10)-C(11)-H(11)	113.3
C(12)-C(11)-H(11)	113.3
C(16)-C(11)-H(11)	113.3
O(9)-C(12)-C(13)	108.7(4)
O(9)-C(12)-C(11)	113.2(3)
C(13)-C(12)-C(11)	104.2(4)
O(9)-C(12)-H(12)	110.2
C(13)-C(12)-H(12)	110.2
C(11)-C(12)-H(12)	110.2
C(14)-C(13)-C(12)	106.7(4)
C(14)-C(13)-C(9)	61.0(3)
C(12)-C(13)-C(9)	107.9(4)
C(14)-C(13)-H(13)	121.9
C(12)-C(13)-H(13)	121.9
C(9)-C(13)-H(13)	121.9
C(13)-C(14)-C(15)	112.3(4)
C(13)-C(14)-C(9)	60.7(3)
C(15)-C(14)-C(9)	123.1(4)
C(13)-C(14)-H(14)	116.1
C(15)-C(14)-H(14)	116.1
C(9)-C(14)-H(14)	116.1
C(16)-C(15)-C(14)	109.9(4)
C(16)-C(15)-C(20)	106.1(4)
C(14)-C(15)-C(20)	107.5(4)
C(16)-C(15)-H(15)	111.0
C(14)-C(15)-H(15)	111.0
C(20)-C(15)-H(15)	111.0

C(17)-C(16)-C(15)	113.5(4)
C(17)-C(16)-C(11)	112.5(4)
C(15)-C(16)-C(11)	105.3(3)
C(17)-C(16)-H(16)	108.4
C(15)-C(16)-H(16)	108.4
C(11)-C(16)-H(16)	108.4
C(18)-C(17)-C(16)	124.2(4)
C(18)-C(17)-H(17)	117.9
C(16)-C(17)-H(17)	117.9
C(17)-C(18)-C(19)	120.7(4)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
O(8)-C(19)-C(18)	123.5(5)
O(8)-C(19)-C(20)	120.8(5)
C(18)-C(19)-C(20)	115.5(4)
O(9)-C(20)-C(21)	105.4(4)
O(9)-C(20)-C(19)	103.2(3)
C(21)-C(20)-C(19)	111.0(4)
O(9)-C(20)-C(15)	109.1(3)
C(21)-C(20)-C(15)	114.6(4)
C(19)-C(20)-C(15)	112.6(4)
O(10A)-C(21)-C(20)	107.7(10)
C(20)-C(21)-O(10)	106.2(4)
C(20)-C(21)-H(21A)	110.5
O(10)-C(21)-H(21A)	110.5
C(20)-C(21)-H(21B)	110.5
O(10)-C(21)-H(21B)	110.5
H(21A)-C(21)-H(21B)	108.7
O(10A)-C(21)-H(21C)	110.2
C(20)-C(21)-H(21C)	110.2
O(10A)-C(21)-H(21D)	110.2
C(20)-C(21)-H(21D)	110.2
H(21C)-C(21)-H(21D)	108.5
O(11)-S(1)-O(12)	121.8(5)
O(11)-S(1)-O(10)	112.7(4)
O(12)-S(1)-O(10)	107.3(5)
O(11)-S(1)-C(22)	107.0(4)
O(12)-S(1)-C(22)	104.7(4)

O(10)-S(1)-C(22)	101.2(4)
S(1)-O(10)-C(21)	119.5(5)
F(1)-C(22)-F(3)	110.9(8)
F(1)-C(22)-F(2)	108.6(8)
F(3)-C(22)-F(2)	107.1(7)
F(1)-C(22)-S(1)	111.6(6)
F(3)-C(22)-S(1)	107.7(6)
F(2)-C(22)-S(1)	110.9(5)
O(12A)-S(1A)-O(10A)	106(2)
O(12A)-S(1A)-O(11A)	122(2)
O(10A)-S(1A)-O(11A)	107(2)
O(12A)-S(1A)-C(22A)	99(2)
O(10A)-S(1A)-C(22A)	118.5(13)
O(11A)-S(1A)-C(22A)	106(2)
C(21)-O(10A)-S(1A)	123.8(17)
F(1A)-C(22A)-F(2A)	93(2)
F(1A)-C(22A)-F(3)	120(3)
F(2A)-C(22A)-F(3)	133(3)
F(1A)-C(22A)-S(1A)	103(2)
F(2A)-C(22A)-S(1A)	98.1(18)
F(3)-C(22A)-S(1A)	105.0(13)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17sel4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	36(2)	105(4)	27(2)	-12(3)	-8(2)	20(3)
N(2)	36(2)	48(3)	48(3)	8(2)	6(2)	4(2)
O(1)	40(2)	39(2)	24(1)	-4(1)	-7(1)	-9(1)
O(2)	45(2)	55(2)	41(2)	-15(2)	1(2)	-22(2)
O(3)	59(3)	98(4)	44(2)	-32(2)	-22(2)	8(3)
O(4)	57(3)	132(5)	26(2)	-4(2)	-6(2)	12(3)
O(5)	54(2)	62(3)	57(2)	20(2)	13(2)	12(2)
O(6)	53(2)	67(3)	49(2)	1(2)	1(2)	-13(2)
O(7)	41(2)	34(2)	40(2)	-1(1)	6(1)	1(2)
O(8)	51(2)	57(2)	51(2)	-9(2)	12(2)	10(2)
O(9)	31(2)	36(2)	33(2)	-2(1)	5(1)	-2(1)
C(1)	26(2)	47(3)	30(2)	-10(2)	-4(2)	-4(2)
C(2)	25(2)	50(3)	28(2)	-6(2)	-4(2)	4(2)
C(3)	26(2)	59(3)	30(2)	-11(2)	-7(2)	7(2)
C(4)	25(2)	77(4)	28(2)	-9(2)	-8(2)	13(2)
C(5)	30(2)	68(4)	29(2)	6(2)	1(2)	16(2)
C(6)	26(2)	46(3)	38(2)	2(2)	2(2)	10(2)
C(7)	26(2)	41(3)	28(2)	-5(2)	-4(2)	3(2)
C(8)	58(3)	40(3)	30(2)	1(2)	-6(2)	-18(2)
C(9)	38(2)	38(2)	25(2)	-3(2)	-3(2)	-7(2)
C(10)	33(2)	33(2)	26(2)	6(2)	1(2)	-6(2)
C(11)	27(2)	40(2)	26(2)	-3(2)	-4(2)	-5(2)
C(12)	28(2)	33(2)	29(2)	-2(2)	1(2)	-1(2)
C(13)	35(2)	36(2)	24(2)	2(2)	-2(2)	-9(2)
C(14)	27(2)	37(2)	30(2)	3(2)	-5(2)	-8(2)
C(15)	26(2)	37(2)	30(2)	3(2)	-1(2)	-6(2)
C(16)	29(2)	46(3)	25(2)	4(2)	-1(2)	-1(2)
C(17)	35(2)	66(3)	25(2)	1(2)	-5(2)	5(2)
C(18)	39(3)	62(3)	28(2)	-6(2)	1(2)	-3(2)
C(19)	31(2)	50(3)	35(2)	-3(2)	8(2)	-8(2)
C(20)	25(2)	39(2)	30(2)	2(2)	2(2)	-1(2)
C(21)	28(2)	51(3)	41(3)	6(2)	6(2)	0(2)
S(1)	27(1)	52(1)	44(1)	4(1)	-5(1)	-2(1)

O(10)	25(3)	34(4)	45(3)	7(3)	-9(2)	-9(3)
O(11)	43(3)	57(4)	83(5)	15(3)	4(3)	6(3)
O(12)	35(3)	69(4)	56(4)	-5(3)	12(3)	-7(3)
C(22)	46(5)	74(6)	54(5)	1(4)	-17(4)	-16(4)
F(1)	140(7)	71(4)	78(4)	-15(3)	-11(4)	-40(4)
F(2)	89(4)	162(7)	41(3)	-7(3)	1(3)	-56(5)
S(1A)	90(6)	91(6)	128(7)	-14(5)	28(5)	-19(5)
O(10A)	36(7)	66(11)	52(8)	15(8)	4(6)	-19(7)
O(11A)	160(20)	170(20)	220(20)	-39(17)	43(17)	21(17)
O(12A)	109(17)	140(20)	122(19)	15(15)	56(14)	-19(15)
C(22A)	148(19)	147(19)	150(20)	-3(10)	11(10)	-2(10)
F(1A)	139(16)	160(16)	131(15)	-1(13)	13(13)	22(14)
F(2A)	146(17)	191(19)	184(19)	0(16)	10(15)	46(15)
F(3)	65(3)	252(8)	95(4)	-7(5)	-32(3)	-17(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17sel4.

	x	y	z	U(eq)
H(3)	2003	7913	7711	47
H(5)	1165	2490	8566	51
H(7)	882	3267	6609	38
H(8A)	1975	7941	5360	51
H(8B)	1137	8714	5304	51
H(11)	112	3510	3780	38
H(12)	636	1293	4621	36
H(13)	1727	2728	5255	38
H(14)	2454	5279	4625	38
H(15)	2260	5067	3474	37
H(16)	1063	6356	3372	40
H(17)	549	4151	2527	51
H(18)	1205	1328	2151	52
H(21A)	2769	-722	3923	48
H(21B)	2699	1079	4490	48
H(21C)	2776	1531	4454	48
H(21D)	2686	-759	4058	48

Table 7. Torsion angles [°] for s17sel4.

C(8)-O(1)-C(1)-O(2)	4.0(7)
C(8)-O(1)-C(1)-C(2)	-177.2(4)
O(2)-C(1)-C(2)-C(7)	173.2(4)
O(1)-C(1)-C(2)-C(7)	-5.6(6)
O(2)-C(1)-C(2)-C(3)	-5.8(7)
O(1)-C(1)-C(2)-C(3)	175.5(4)
C(7)-C(2)-C(3)-C(4)	-0.6(7)
C(1)-C(2)-C(3)-C(4)	178.4(4)
C(2)-C(3)-C(4)-C(5)	1.1(7)
C(2)-C(3)-C(4)-N(1)	-178.3(4)
O(3)-N(1)-C(4)-C(5)	-172.1(5)
O(4)-N(1)-C(4)-C(5)	8.6(7)
O(3)-N(1)-C(4)-C(3)	7.3(7)
O(4)-N(1)-C(4)-C(3)	-172.1(5)
C(3)-C(4)-C(5)-C(6)	-1.5(7)
N(1)-C(4)-C(5)-C(6)	177.9(4)
C(4)-C(5)-C(6)-C(7)	1.5(7)
C(4)-C(5)-C(6)-N(2)	179.7(4)
O(6)-N(2)-C(6)-C(7)	-6.2(6)
O(5)-N(2)-C(6)-C(7)	172.6(4)
O(6)-N(2)-C(6)-C(5)	175.4(5)
O(5)-N(2)-C(6)-C(5)	-5.8(6)
C(5)-C(6)-C(7)-C(2)	-1.0(7)
N(2)-C(6)-C(7)-C(2)	-179.3(4)
C(3)-C(2)-C(7)-C(6)	0.5(6)
C(1)-C(2)-C(7)-C(6)	-178.4(4)
C(1)-O(1)-C(8)-C(9)	167.2(4)
O(1)-C(8)-C(9)-C(10)	97.1(5)
O(1)-C(8)-C(9)-C(13)	-36.9(6)
O(1)-C(8)-C(9)-C(14)	-106.0(5)
C(8)-C(9)-C(10)-O(7)	5.4(7)
C(13)-C(9)-C(10)-O(7)	146.2(4)
C(14)-C(9)-C(10)-O(7)	-152.3(4)
C(8)-C(9)-C(10)-C(11)	-173.0(4)
C(13)-C(9)-C(10)-C(11)	-32.3(4)
C(14)-C(9)-C(10)-C(11)	29.2(5)

O(7)-C(10)-C(11)-C(12)	-138.8(4)
C(9)-C(10)-C(11)-C(12)	39.6(4)
O(7)-C(10)-C(11)-C(16)	107.8(5)
C(9)-C(10)-C(11)-C(16)	-73.8(4)
C(20)-O(9)-C(12)-C(13)	-53.8(5)
C(20)-O(9)-C(12)-C(11)	61.5(4)
C(10)-C(11)-C(12)-O(9)	-148.6(3)
C(16)-C(11)-C(12)-O(9)	-38.4(5)
C(10)-C(11)-C(12)-C(13)	-30.7(4)
C(16)-C(11)-C(12)-C(13)	79.6(4)
O(9)-C(12)-C(13)-C(14)	68.3(5)
C(11)-C(12)-C(13)-C(14)	-52.7(5)
O(9)-C(12)-C(13)-C(9)	132.5(4)
C(11)-C(12)-C(13)-C(9)	11.5(5)
C(10)-C(9)-C(13)-C(14)	112.1(4)
C(8)-C(9)-C(13)-C(14)	-107.9(5)
C(10)-C(9)-C(13)-C(12)	12.5(5)
C(8)-C(9)-C(13)-C(12)	152.5(4)
C(14)-C(9)-C(13)-C(12)	-99.6(4)
C(12)-C(13)-C(14)-C(15)	-14.9(5)
C(9)-C(13)-C(14)-C(15)	-116.5(4)
C(12)-C(13)-C(14)-C(9)	101.6(4)
C(10)-C(9)-C(14)-C(13)	-91.4(4)
C(8)-C(9)-C(14)-C(13)	110.9(5)
C(10)-C(9)-C(14)-C(15)	7.5(6)
C(8)-C(9)-C(14)-C(15)	-150.3(4)
C(13)-C(9)-C(14)-C(15)	98.9(5)
C(13)-C(14)-C(15)-C(16)	68.2(5)
C(9)-C(14)-C(15)-C(16)	-0.4(6)
C(13)-C(14)-C(15)-C(20)	-46.9(5)
C(9)-C(14)-C(15)-C(20)	-115.5(4)
C(14)-C(15)-C(16)-C(17)	-164.4(4)
C(20)-C(15)-C(16)-C(17)	-48.5(5)
C(14)-C(15)-C(16)-C(11)	-40.9(5)
C(20)-C(15)-C(16)-C(11)	75.0(4)
C(10)-C(11)-C(16)-C(17)	-153.3(4)
C(12)-C(11)-C(16)-C(17)	97.4(4)
C(10)-C(11)-C(16)-C(15)	82.6(4)

C(12)-C(11)-C(16)-C(15)	-26.8(5)
C(15)-C(16)-C(17)-C(18)	18.9(7)
C(11)-C(16)-C(17)-C(18)	-100.6(6)
C(16)-C(17)-C(18)-C(19)	4.6(8)
C(17)-C(18)-C(19)-O(8)	-179.6(5)
C(17)-C(18)-C(19)-C(20)	5.7(7)
C(12)-O(9)-C(20)-C(21)	111.9(4)
C(12)-O(9)-C(20)-C(19)	-131.6(4)
C(12)-O(9)-C(20)-C(15)	-11.7(5)
O(8)-C(19)-C(20)-O(9)	-96.3(5)
C(18)-C(19)-C(20)-O(9)	78.5(5)
O(8)-C(19)-C(20)-C(21)	16.2(6)
C(18)-C(19)-C(20)-C(21)	-169.1(4)
O(8)-C(19)-C(20)-C(15)	146.2(5)
C(18)-C(19)-C(20)-C(15)	-39.0(6)
C(16)-C(15)-C(20)-O(9)	-55.0(4)
C(14)-C(15)-C(20)-O(9)	62.6(4)
C(16)-C(15)-C(20)-C(21)	-172.8(4)
C(14)-C(15)-C(20)-C(21)	-55.3(5)
C(16)-C(15)-C(20)-C(19)	59.0(5)
C(14)-C(15)-C(20)-C(19)	176.6(3)
O(9)-C(20)-C(21)-O(10A)	167.0(10)
C(19)-C(20)-C(21)-O(10A)	55.9(10)
C(15)-C(20)-C(21)-O(10A)	-73.0(10)
O(9)-C(20)-C(21)-O(10)	-173.0(4)
C(19)-C(20)-C(21)-O(10)	76.0(6)
C(15)-C(20)-C(21)-O(10)	-53.0(6)
O(11)-S(1)-O(10)-C(21)	12.4(8)
O(12)-S(1)-O(10)-C(21)	149.1(6)
C(22)-S(1)-O(10)-C(21)	-101.5(6)
C(20)-C(21)-O(10)-S(1)	-157.1(5)
O(11)-S(1)-C(22)-F(1)	-177.7(7)
O(12)-S(1)-C(22)-F(1)	51.8(8)
O(10)-S(1)-C(22)-F(1)	-59.6(8)
O(11)-S(1)-C(22)-F(3)	60.4(7)
O(12)-S(1)-C(22)-F(3)	-70.1(7)
O(10)-S(1)-C(22)-F(3)	178.5(6)
O(11)-S(1)-C(22)-F(2)	-56.5(7)

O(12)-S(1)-C(22)-F(2)	173.0(7)
O(10)-S(1)-C(22)-F(2)	61.6(7)
C(20)-C(21)-O(10A)-S(1A)	133.9(18)
O(12A)-S(1A)-O(10A)-C(21)	-176(2)
O(11A)-S(1A)-O(10A)-C(21)	-45(3)
C(22A)-S(1A)-O(10A)-C(21)	75(3)
O(12A)-S(1A)-C(22A)-F(1A)	-58(2)
O(10A)-S(1A)-C(22A)-F(1A)	55(3)
O(11A)-S(1A)-C(22A)-F(1A)	175(2)
O(12A)-S(1A)-C(22A)-F(2A)	-152(2)
O(10A)-S(1A)-C(22A)-F(2A)	-39(3)
O(11A)-S(1A)-C(22A)-F(2A)	81(3)
O(12A)-S(1A)-C(22A)-F(3)	69(2)
O(10A)-S(1A)-C(22A)-F(3)	-177.9(18)
O(11A)-S(1A)-C(22A)-F(3)	-58(3)

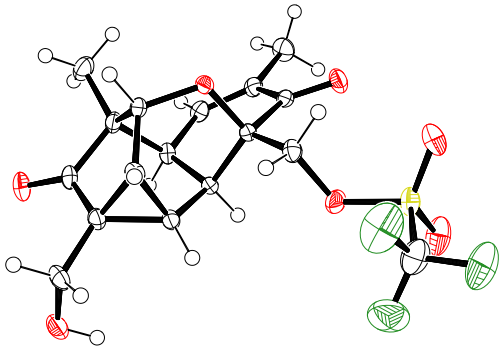


Table 1. Crystal data and structure refinement for s18sel1.

Identification code	s18sel1	
Empirical formula	C17 H17 F3 O7 S	
Formula weight	422.36	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 9.86890(10) Å	α= 90°.
	b = 10.31940(10) Å	β= 90°.
	c = 34.7360(5) Å	γ = 90°.
Volume	3537.55(7) Å^3	
Z	8	

Density (calculated)	1.586 Mg/m^3
Absorption coefficient	2.291 mm^{-1}
F(000)	1744
Crystal size	0.250 x 0.150 x 0.030 mm^3
Theta range for data collection	2.544 to 73.017°.
Index ranges	-12<=h<=11, -10<=k<=12, -42<=l<=42
Reflections collected	33311
Independent reflections	3537 [R(int) = 0.0547]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.73393
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3537 / 0 / 259
Goodness-of-fit on F^2	1.157
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1354
R indices (all data)	R1 = 0.0551, wR2 = 0.1378
Extinction coefficient	n/a
Largest diff. peak and hole	0.823 and -0.552 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18sel1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S	9602(1)	6139(1)	2942(1)	25(1)
O(1)	10153(2)	4918(2)	2853(1)	42(1)
O(2)	10405(2)	7196(2)	3056(1)	43(1)
O(3)	8408(2)	6049(2)	3231(1)	25(1)
O(4)	9797(2)	4152(2)	3748(1)	25(1)
O(5)	6661(2)	3495(2)	3755(1)	18(1)
O(6)	3122(2)	5332(2)	4517(1)	28(1)
O(7)	2692(2)	7778(2)	3918(1)	32(1)
F(1)	8047(3)	7740(2)	2569(1)	64(1)
F(2)	7836(2)	5743(3)	2407(1)	65(1)
F(3)	9588(3)	6830(3)	2228(1)	62(1)
C(1)	8698(3)	6656(3)	2511(1)	39(1)
C(2)	7675(2)	4830(2)	3289(1)	20(1)
C(3)	7429(2)	4674(2)	3720(1)	15(1)
C(4)	8772(2)	4402(2)	3930(1)	17(1)
C(5)	8737(2)	4391(2)	4353(1)	19(1)
C(6)	9976(3)	3936(3)	4561(1)	26(1)
C(7)	7596(2)	4780(2)	4529(1)	20(1)
C(8)	6369(2)	5293(2)	4327(1)	17(1)
C(9)	6658(2)	5780(2)	3917(1)	15(1)
C(10)	5335(2)	5989(2)	3696(1)	17(1)
C(12)	5267(2)	3714(2)	3872(1)	18(1)
C(13)	5185(2)	4276(2)	4285(1)	19(1)
C(14)	5108(3)	3263(3)	4600(1)	28(1)
C(15)	3950(2)	5152(2)	4264(1)	20(1)
C(16)	3934(2)	5738(2)	3874(1)	19(1)
C(17)	2749(2)	6542(3)	3739(1)	25(1)
C(18)	4616(2)	4735(2)	3618(1)	18(1)

Table 3. Bond lengths [Å] for s18sel1.

S-O(2)	1.406(2)
S-O(1)	1.406(2)
S-O(3)	1.5510(17)
S-C(1)	1.824(3)
O(3)-C(2)	1.465(3)
O(4)-C(4)	1.222(3)
O(5)-C(3)	1.439(3)
O(5)-C(12)	1.452(3)
O(6)-C(15)	1.214(3)
O(7)-C(17)	1.421(3)
O(7)-H(7A)	0.88(5)
F(1)-C(1)	1.306(4)
F(2)-C(1)	1.320(4)
F(3)-C(1)	1.330(4)
C(2)-C(3)	1.524(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(9)	1.534(3)
C(3)-C(4)	1.539(3)
C(4)-C(5)	1.467(3)
C(5)-C(7)	1.343(3)
C(5)-C(6)	1.498(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(8)	1.495(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.537(3)
C(8)-C(13)	1.578(3)
C(8)-H(8)	1.0000
C(9)-C(10)	1.529(3)
C(9)-H(9)	1.0000
C(10)-C(18)	1.500(3)
C(10)-C(16)	1.536(3)
C(10)-H(10)	1.0000
C(12)-C(18)	1.516(3)

C(12)-C(13)	1.552(3)
C(12)-H(12)	1.0000
C(13)-C(14)	1.515(3)
C(13)-C(15)	1.519(3)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.482(3)
C(16)-C(17)	1.509(3)
C(16)-C(18)	1.523(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18)	1.0000

Table 4. Bond angles [°] for s18sel1.

O(2)-S-O(1)	122.60(15)
O(2)-S-O(3)	107.01(12)
O(1)-S-O(3)	112.53(12)
O(2)-S-C(1)	106.22(15)
O(1)-S-C(1)	105.72(15)
O(3)-S-C(1)	100.25(13)
C(2)-O(3)-S	121.02(15)
C(3)-O(5)-C(12)	113.06(16)
C(17)-O(7)-H(7A)	107(3)
F(1)-C(1)-F(2)	109.7(3)
F(1)-C(1)-F(3)	108.9(3)
F(2)-C(1)-F(3)	108.7(3)
F(1)-C(1)-S	111.4(2)
F(2)-C(1)-S	109.3(2)
F(3)-C(1)-S	108.8(2)
O(3)-C(2)-C(3)	107.74(18)
O(3)-C(2)-H(2A)	110.2
C(3)-C(2)-H(2A)	110.2
O(3)-C(2)-H(2B)	110.2
C(3)-C(2)-H(2B)	110.2
H(2A)-C(2)-H(2B)	108.5
O(5)-C(3)-C(2)	104.84(17)
O(5)-C(3)-C(9)	109.25(17)
C(2)-C(3)-C(9)	116.04(18)
O(5)-C(3)-C(4)	105.05(17)
C(2)-C(3)-C(4)	110.39(18)
C(9)-C(3)-C(4)	110.55(18)
O(4)-C(4)-C(5)	122.5(2)
O(4)-C(4)-C(3)	120.3(2)
C(5)-C(4)-C(3)	117.10(19)
C(7)-C(5)-C(4)	118.2(2)
C(7)-C(5)-C(6)	124.0(2)
C(4)-C(5)-C(6)	117.8(2)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5

C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-C(8)	124.9(2)
C(5)-C(7)-H(7)	117.6
C(8)-C(7)-H(7)	117.6
C(7)-C(8)-C(9)	113.56(18)
C(7)-C(8)-C(13)	114.03(19)
C(9)-C(8)-C(13)	105.61(17)
C(7)-C(8)-H(8)	107.8
C(9)-C(8)-H(8)	107.8
C(13)-C(8)-H(8)	107.8
C(10)-C(9)-C(3)	107.71(18)
C(10)-C(9)-C(8)	110.65(18)
C(3)-C(9)-C(8)	105.22(17)
C(10)-C(9)-H(9)	111.0
C(3)-C(9)-H(9)	111.0
C(8)-C(9)-H(9)	111.0
C(18)-C(10)-C(9)	111.96(19)
C(18)-C(10)-C(16)	60.20(15)
C(9)-C(10)-C(16)	122.87(19)
C(18)-C(10)-H(10)	116.3
C(9)-C(10)-H(10)	116.3
C(16)-C(10)-H(10)	116.3
O(5)-C(12)-C(18)	110.33(18)
O(5)-C(12)-C(13)	111.45(18)
C(18)-C(12)-C(13)	104.88(19)
O(5)-C(12)-H(12)	110.0
C(18)-C(12)-H(12)	110.0
C(13)-C(12)-H(12)	110.0
C(14)-C(13)-C(15)	113.9(2)
C(14)-C(13)-C(12)	114.4(2)
C(15)-C(13)-C(12)	102.63(18)
C(14)-C(13)-C(8)	115.4(2)
C(15)-C(13)-C(8)	101.74(18)
C(12)-C(13)-C(8)	107.19(17)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5

H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(6)-C(15)-C(16)	126.2(2)
O(6)-C(15)-C(13)	126.6(2)
C(16)-C(15)-C(13)	107.21(19)
C(15)-C(16)-C(17)	121.2(2)
C(15)-C(16)-C(18)	104.60(19)
C(17)-C(16)-C(18)	122.2(2)
C(15)-C(16)-C(10)	115.24(19)
C(17)-C(16)-C(10)	118.6(2)
C(18)-C(16)-C(10)	58.73(15)
O(7)-C(17)-C(16)	112.8(2)
O(7)-C(17)-H(17A)	109.0
C(16)-C(17)-H(17A)	109.0
O(7)-C(17)-H(17B)	109.0
C(16)-C(17)-H(17B)	109.0
H(17A)-C(17)-H(17B)	107.8
C(10)-C(18)-C(12)	107.02(18)
C(10)-C(18)-C(16)	61.07(15)
C(12)-C(18)-C(16)	108.61(19)
C(10)-C(18)-H(18)	121.6
C(12)-C(18)-H(18)	121.6
C(16)-C(18)-H(18)	121.6

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18sel1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S	21(1)	36(1)	20(1)	-3(1)	4(1)	-3(1)
O(1)	34(1)	45(1)	47(1)	-3(1)	17(1)	10(1)
O(2)	37(1)	58(1)	33(1)	-11(1)	5(1)	-21(1)
O(3)	29(1)	23(1)	22(1)	0(1)	10(1)	-1(1)
O(4)	15(1)	32(1)	28(1)	0(1)	4(1)	4(1)
O(5)	13(1)	14(1)	26(1)	-2(1)	0(1)	-1(1)
O(6)	18(1)	42(1)	26(1)	-2(1)	8(1)	-1(1)
O(7)	17(1)	26(1)	51(1)	-4(1)	1(1)	4(1)
F(1)	79(2)	66(1)	48(1)	18(1)	1(1)	26(1)
F(2)	61(1)	89(2)	44(1)	0(1)	-23(1)	-28(1)
F(3)	77(2)	85(2)	22(1)	4(1)	17(1)	-15(1)
C(1)	43(2)	51(2)	22(1)	3(1)	1(1)	-8(2)
C(2)	19(1)	22(1)	20(1)	-3(1)	3(1)	-1(1)
C(3)	13(1)	14(1)	18(1)	0(1)	1(1)	0(1)
C(4)	13(1)	14(1)	24(1)	1(1)	0(1)	-1(1)
C(5)	15(1)	20(1)	22(1)	1(1)	-3(1)	-3(1)
C(6)	20(1)	33(1)	27(1)	2(1)	-6(1)	1(1)
C(7)	19(1)	23(1)	17(1)	1(1)	-2(1)	-4(1)
C(8)	14(1)	22(1)	16(1)	-2(1)	2(1)	-2(1)
C(9)	14(1)	14(1)	16(1)	0(1)	1(1)	1(1)
C(10)	15(1)	19(1)	18(1)	1(1)	2(1)	2(1)
C(12)	12(1)	17(1)	25(1)	1(1)	0(1)	-3(1)
C(13)	15(1)	22(1)	20(1)	3(1)	3(1)	-2(1)
C(14)	25(1)	31(1)	27(1)	11(1)	2(1)	-4(1)
C(15)	12(1)	25(1)	22(1)	-2(1)	2(1)	-4(1)
C(16)	14(1)	22(1)	22(1)	0(1)	1(1)	0(1)
C(17)	14(1)	30(1)	31(1)	-2(1)	-2(1)	4(1)
C(18)	16(1)	19(1)	20(1)	-2(1)	-1(1)	1(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s18sel1.

	x	y	z	U(eq)
H(7A)	3450(50)	8190(40)	3861(12)	57(12)
H(2A)	8216	4094	3191	24
H(2B)	6800	4850	3150	24
H(6A)	9787	3891	4838	40
H(6B)	10722	4544	4515	40
H(6C)	10232	3074	4467	40
H(7)	7565	4724	4801	24
H(8)	6018	6041	4481	21
H(9)	7212	6591	3922	18
H(10)	5367	6624	3479	21
H(12)	4742	2887	3856	22
H(14A)	4264	2770	4574	41
H(14B)	5129	3690	4852	41
H(14C)	5883	2673	4578	41
H(17A)	2815	6660	3456	30
H(17B)	1898	6068	3793	30
H(18)	4255	4521	3356	22

Table 7. Torsion angles [°] for s18sel1.

O(2)-S-O(3)-C(2)	-157.23(19)
O(1)-S-O(3)-C(2)	-19.8(2)
C(1)-S-O(3)-C(2)	92.1(2)
O(2)-S-C(1)-F(1)	-53.4(3)
O(1)-S-C(1)-F(1)	174.9(2)
O(3)-S-C(1)-F(1)	57.8(2)
O(2)-S-C(1)-F(2)	-174.8(2)
O(1)-S-C(1)-F(2)	53.5(3)
O(3)-S-C(1)-F(2)	-63.5(2)
O(2)-S-C(1)-F(3)	66.6(3)
O(1)-S-C(1)-F(3)	-65.1(3)
O(3)-S-C(1)-F(3)	177.9(2)
S-O(3)-C(2)-C(3)	137.92(17)
C(12)-O(5)-C(3)-C(2)	-110.24(19)
C(12)-O(5)-C(3)-C(9)	14.8(2)
C(12)-O(5)-C(3)-C(4)	133.37(18)
O(3)-C(2)-C(3)-O(5)	177.61(17)
O(3)-C(2)-C(3)-C(9)	57.0(2)
O(3)-C(2)-C(3)-C(4)	-69.7(2)
O(5)-C(3)-C(4)-O(4)	101.8(2)
C(2)-C(3)-C(4)-O(4)	-10.7(3)
C(9)-C(3)-C(4)-O(4)	-140.4(2)
O(5)-C(3)-C(4)-C(5)	-75.0(2)
C(2)-C(3)-C(4)-C(5)	172.45(19)
C(9)-C(3)-C(4)-C(5)	42.7(3)
O(4)-C(4)-C(5)-C(7)	174.7(2)
C(3)-C(4)-C(5)-C(7)	-8.5(3)
O(4)-C(4)-C(5)-C(6)	-5.7(3)
C(3)-C(4)-C(5)-C(6)	171.1(2)
C(4)-C(5)-C(7)-C(8)	-3.3(4)
C(6)-C(5)-C(7)-C(8)	177.1(2)
C(5)-C(7)-C(8)-C(9)	-19.7(3)
C(5)-C(7)-C(8)-C(13)	101.4(3)
O(5)-C(3)-C(9)-C(10)	-64.3(2)
C(2)-C(3)-C(9)-C(10)	53.8(2)
C(4)-C(3)-C(9)-C(10)	-179.47(17)

O(5)-C(3)-C(9)-C(8)	53.7(2)
C(2)-C(3)-C(9)-C(8)	171.92(18)
C(4)-C(3)-C(9)-C(8)	-61.4(2)
C(7)-C(8)-C(9)-C(10)	166.66(19)
C(13)-C(8)-C(9)-C(10)	41.0(2)
C(7)-C(8)-C(9)-C(3)	50.6(2)
C(13)-C(8)-C(9)-C(3)	-75.1(2)
C(3)-C(9)-C(10)-C(18)	47.0(2)
C(8)-C(9)-C(10)-C(18)	-67.5(2)
C(3)-C(9)-C(10)-C(16)	114.9(2)
C(8)-C(9)-C(10)-C(16)	0.4(3)
C(3)-O(5)-C(12)-C(18)	50.5(2)
C(3)-O(5)-C(12)-C(13)	-65.6(2)
O(5)-C(12)-C(13)-C(14)	-89.3(2)
C(18)-C(12)-C(13)-C(14)	151.3(2)
O(5)-C(12)-C(13)-C(15)	146.74(18)
C(18)-C(12)-C(13)-C(15)	27.4(2)
O(5)-C(12)-C(13)-C(8)	40.0(2)
C(18)-C(12)-C(13)-C(8)	-79.4(2)
C(7)-C(8)-C(13)-C(14)	29.6(3)
C(9)-C(8)-C(13)-C(14)	155.0(2)
C(7)-C(8)-C(13)-C(15)	153.52(19)
C(9)-C(8)-C(13)-C(15)	-81.1(2)
C(7)-C(8)-C(13)-C(12)	-99.1(2)
C(9)-C(8)-C(13)-C(12)	26.3(2)
C(14)-C(13)-C(15)-O(6)	19.5(4)
C(12)-C(13)-C(15)-O(6)	143.8(2)
C(8)-C(13)-C(15)-O(6)	-105.3(3)
C(14)-C(13)-C(15)-C(16)	-160.0(2)
C(12)-C(13)-C(15)-C(16)	-35.7(2)
C(8)-C(13)-C(15)-C(16)	75.2(2)
O(6)-C(15)-C(16)-C(17)	-6.8(4)
C(13)-C(15)-C(16)-C(17)	172.7(2)
O(6)-C(15)-C(16)-C(18)	-150.1(2)
C(13)-C(15)-C(16)-C(18)	29.4(2)
O(6)-C(15)-C(16)-C(10)	148.0(2)
C(13)-C(15)-C(16)-C(10)	-32.5(3)
C(18)-C(10)-C(16)-C(15)	92.3(2)

C(9)-C(10)-C(16)-C(15)	-5.9(3)
C(18)-C(10)-C(16)-C(17)	-112.3(2)
C(9)-C(10)-C(16)-C(17)	149.5(2)
C(9)-C(10)-C(16)-C(18)	-98.2(2)
C(15)-C(16)-C(17)-O(7)	72.8(3)
C(18)-C(16)-C(17)-O(7)	-150.3(2)
C(10)-C(16)-C(17)-O(7)	-81.2(3)
C(9)-C(10)-C(18)-C(12)	14.1(2)
C(16)-C(10)-C(18)-C(12)	-102.2(2)
C(9)-C(10)-C(18)-C(16)	116.3(2)
O(5)-C(12)-C(18)-C(10)	-66.0(2)
C(13)-C(12)-C(18)-C(10)	54.1(2)
O(5)-C(12)-C(18)-C(16)	-130.49(19)
C(13)-C(12)-C(18)-C(16)	-10.4(2)
C(15)-C(16)-C(18)-C(10)	-110.9(2)
C(17)-C(16)-C(18)-C(10)	106.3(2)
C(15)-C(16)-C(18)-C(12)	-11.3(2)
C(17)-C(16)-C(18)-C(12)	-154.1(2)
C(10)-C(16)-C(18)-C(12)	99.6(2)

Table 8. Hydrogen bonds for s18sel1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(7A)...O(4)#1	0.88(5)	2.03(5)	2.915(3)	178(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,z

7.3: Computational methodology

DFT calculations were run with Gaussian 09 (Revision D.01),[1] all atoms were described with the 6-31G** basis set, with the exception of S where SDDALL was employed with an additional *d* function (0.503) (BS1).[2] Initial BP86[3] optimizations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as minima (all positive eigenvalues). All energies were recomputed with a larger basis set; 6-311++G** (BS2). Corrections for the effect of DCM (ε = 8.93) solvent were run using the polarizable continuum model and BS1.[4] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[5]

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